Open Notebook Science Melting Points

Open Data Melting Points

of

Organic Compounds

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First Edition: August 11, 2011

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Preface

Introduction

This book represents a PDF version of Dataset ONSMP029 from a project to collect and curate melting points made available as Open Data.(1,2) This particular collection was selected from the application of a threshold to favor the likelihood of reliability. Specifically, the entire range of averaged values for a data point was set to 0.01 C to 5 C, with at least two different measurements within this range. Since provenance information for melting points from various sources is rarely provided, identical values are assumed to ultimately arise from the same origin (thus the requirement for at least 0.01 C difference).

Curators

Jean-Claude Bradley, Andrew Lang, Antony Williams and Evan Curtin.

Data Sources

Measurements were pooled and processed from the following sources: Alfa Aesar (3,4,5), MDPI (5, 6), Bergstrom(4,7), PhysProp(8,9), DrugBank(10), Bell(11), Oxford MSDS(12), Hughes(13), Griffiths(14) and the Chemical Information Validation Spreadsheet(15,16). Links to all the information sources are available from the Open Melting Point Collections Index(1).

Data Processing

The curation of this dataset is an ongoing effort and is implemented by the marking of a data point as "DONOTUSE" or entering new melting point measurements in the Chemical Information Validation spreadsheet(8). Both commercial and free sources are consulted until either enough non-identical values are found or all available sources are exhausted. If there is a clear aggregation of values to support a consensus value then data points clearly outside this range are marked as "DONOTUSE" and these are not counted in the averaging or in the new range of values. This labeling is somewhat subjective and includes other factors, such as details provided in peer-reviewed articles and the proximity of boiling points. Since data sources are never deleted others can re-evaluate this curation process for a given compound and make alternative choices for their own purposes.

This dataset represents a snapshot of the entire Open Melting Point Collection taken on July 30, 2011 followed by automatic exclusion of all compounds where the melting point range was > 0.01 C and < 5 C. Further manual curation removed most compounds with stereoisomers, since it can be difficult to know in many cases whether the reported melting point is of a racemic mixture, a diastereomeric mixture or even another stereoisomer (E/Z or R/S). Every effort was also made to avoid salts and inorganic compounds.

Disclaimer

No claim is made that this dataset is error-free. However, by requiring at least a double validation within a small range, it is expected that the likelihood of a large error has been significantly reduced compared to a single-source database of melting points. Over time the continuous curation effort will increase the size of the double validated dataset and remove any existing errors as they are discovered.

Data Presentation

Entries are sorted alphabetically using common names if possible. 2D image rendering is provided by a ChemSpider web service, as are a few descriptors such as molecular weight, predicted density, ACD/LogP, rule of 5 violations, number of hydrogen bond donors, number of hydrogen bond acceptors, and the number of rotatable bonds.(17)

Two decimal places are provided for all melting points for formatting purposes. This does not necessarily reflect the degree of accuracy provided in the original source. The live data for each compound can be accessed using the following URL (changing the CSID as appropriate):
http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=682

Other web services are available from the Open Melting Point resource page.(2)

Acknowledgments

All students from Drexel University and Oral Roberts University who recorded melting points: Keith DeNivo, Arben Kojtari, Siobhan Toal, Chi Nguyen, Hai Truong, Will Stedman, Danielle Fagnani, David Bulger, Michelle Livings, Mark Mangir, James Brooks, Sigrid Williamson, Curtis Kleier, Mirlinda Biba, Byron Forte, Carol Sha, Francisco Guevara, Arti Patel, Jose Rafael Quejada, Diane Liu, Paul DeGregory, Khalid Mirza.

Harold Bell, Department of Chemistry - Emeritus, Virginia Tech and Will Griffiths from ChemRefer who donated their melting point datasets to the public domain.

John Shirley and Aaron Frederick from Alfa Aesar who donated their melting point collection to the public domain.

Bob Boethling and Cathy Fehrenbacher from the EPA and Bill Meylan and Phil Howard from SRC Inc., who assisted with the donation of the PhysProp melting point collection to the public domain.

References

1) Open Melting Point Dataset Index http://onschallenge.wikispaces.com/Open+Melting+Point+Datasets

2) Open Melting Point Resource web site. http://onswebservices.wikispaces.com/meltingpoint

3) Alfa Aesar web site http://www.alfa.com

4) Bradley, J.-C. Alfa Aesar melting point data now openly available, UsefulChem blog (February 21, 2011)

http://usefulchem.blogspot.com/2011/02/alfa-aesar-melting-point-data-now.html

5) Bradley, J.-C. Validating Melting Point Data from Alfa Aesar, EPI and MDPI, UsefulChem blog (March 4, 2011)

http://usefulchem.blogspot.com/2011/03/validating-melting-point-data-from-alfa.html

6) MDPI web site. http://www.mdpi.org/

7) Bergström, CAS Norinder, U Luthman K and Artursson, P Molecular Descriptors Influencing Melting Point and Their Role in Classification of Solid Drugs, J. Chem. Inf. Mod. 43(4) 1177-1185 (2003) http://pubs.acs.org/doi/abs/10.1021/ci020280x

8) Bradley, J.-C. More Open Melting Points from EPI and other sources: on the path to ultimate curation UsefulChem blog (May 25, 2011)
http://usefulchem.blogspot.com/2011/05/more-open-melting-points-from-epi-and.html

9) PhysProp (EPISuite) dataset web site. http://esc.syrres.com/interkow/EpiSuiteData.htm

10) DrugBank dataset web site http://www.drugbank.ca/extractor

11) Bell dataset http://www.colby.edu/chemistry/cmp/cmp.html

12) Oxford MSDS web site http://msds.chem.ox.ac.uk/

13) Huges dataset http://pubs.acs.org/doi/abs/10.1021/ci700307p

14) Melting points collected from IUCr .cif files by Will Griffiths: http://www.iucr.org/

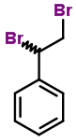
15) Chemical Information Validation web site http://onswebservices.wikispaces.com/ChemInfoValidation

16) Bradley, J.-C. Chemical Information Validation Results from Fall 2010 UsefulChem blog (Jan 5, 2011) http://usefulchem.blogspot.com/2011/01/chemical-information-validation-results.html

17) ChemSpider API web site http://www.chemspider.com/AboutServices.aspx

Melting Points

(1,2-dibromoethyl)benzene C8H8Br2[3, 64]



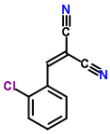
Compound Data

Melting point	**73.50 °C**	**346.65 K**			
CSID	6878	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	263.9571	**H bond donors**	0	**ACD/LogP**	3.69
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.77 g/cm^3
SMILES	BrCC(Br)c1ccccc1				
STD InChIKey	SHKKTLSDGJRCTR-UHFFFAOYAP				

Melting Points

mp °C	source
72.00	Alfa Aesar
75.00	PHYSPROP

(2-chlorobenzylidene)malononitrile C10H5ClN2[61, 64]



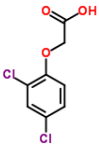
Compound Data

Melting point	**95.25 °C**	**368.40 K**			
CSID	16644	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	188.6131	**H bond donors**	0	**ACD/LogP**	2.35
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	Clc1ccccc1\C=C(/C#N)C#N				
STD InChIKey	JJNZXLAFIPKXIG-UHFFFAOYAA				

Melting Points

mp °C	source
95.00	Oxford University MSDS
95.50	PHYSPROP

(2,4-dichlorophenoxy)acetic acid C8H6Cl2O3[3, 61, 64]



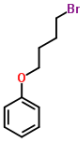
Compound Data

Melting point	**138.83 °C**	**411.98 K**			
CSID	1441	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	221.0374	**H bond donors**	1	**ACD/LogP**	2.58
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.49 g/cm^3
SMILES	Clc1cc(Cl)ccc1OCC(=O)O				
STD InChIKey	OVSKIKFHRZPJSS-UHFFFAOYAM				

Melting Points

mp °C	source
138.00	Alfa Aesar
138.00	Oxford University MSDS
140.50	PHYSPROP

(4-bromobutoxy)benzene C10H13BrO[3, 64]



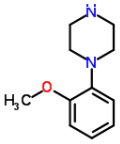
Compound Data

Melting point	**41.50 °C**	**314.65 K**			
CSID	64147	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	229.1136	**H bond donors**	0	**ACD/LogP**	3.72
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.30 g/cm^3
SMILES	BrCCCCOc1ccccc1				
STD InChIKey	QBLISOIWPZSVIK-UHFFFAOYAM				

Melting Points

mp °C	source
42.00	Alfa Aesar
41.00	PHYSPROP

1-(2-methoxyphenyl)piperazine C11H16N2O[3, 64]



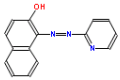
Compound Data

Melting point	**37.75 °C**	**310.90 K**			
CSID	1306	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	192.2575	**H bond donors**	1	**ACD/LogP**	1.13
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	O(c1ccccc1N2CCNCC2)C				
STD InChIKey	VNZLQLYBRIOLFZ-UHFFFAOYAH				

Melting Points

mp °C	source
37.00	Alfa Aesar
38.50	PHYSPROP

1-(2-pyridylazo)-2-naphthol C15H11N3O[3, 61]



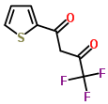
Compound Data

Melting point	**139.75 °C**	**412.90 K**			
CSID	17967090	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	249.2673	**H bond donors**	1	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.24 g/cm^3
SMILES	Oc2ccc3ccccc3c2/N=N/c1ccccn1				
STD InChIKey	LLYOXZQVOKALCD-UHFFFAOYAM				

Melting Points

mp °C	source
140.00	Alfa Aesar
139.50	Oxford University MSDS

1-(2-thenoyl)-3,3,3-trifluoroacetone C8H5F3O2S[3, 32, 64]



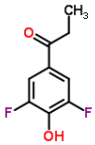
Compound Data

Melting point	**42.33 °C**	**315.48 K**			
CSID	5399	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	222.1843	**H bond donors**	0	**ACD/LogP**	3.76
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.42 g/cm^3
SMILES	O=C(c1sccc1)CC(=O)C(F)(F)F				
STD InChIKey	TXBBUSUXYMIVOS-UHFFFAOYAR				

Melting Points

mp °C	source
43.00	Alfa Aesar
42.00	DrugBank
42.00	PHYSPROP

1-(3,5-difluoro-4-hydroxyphenyl)propan-1-one C9H8F2O2[3, 61]



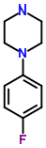
Compound Data

Melting point	**128.50 °C**	**401.65 K**			
CSID	453123	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.1554	**H bond donors**	1	**ACD/LogP**	2.55
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.29 g/cm^3
SMILES	Fc1cc(C(=O)CC)cc(F)c1O				
STD InChIKey	PJIDRPUAOWTRGM-UHFFFAOYAC				

Melting Points

mp °C	source
130.00	Alfa Aesar
127.00	Oxford University MSDS

1-(4-fluorophenyl)piperazine C10H13FN2[3, 64]



Compound Data

Melting point	**31.75 °C**	**304.90 K**			
CSID	67803	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	180.222	**H bond donors**	1	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	Fc1ccc(cc1)N2CCNCC2				
STD InChIKey	AVJKDKWRVSSJPK-UHFFFAOYAS				

Melting Points

mp °C	source
32.00	Alfa Aesar
31.50	PHYSPROP

1-(chloromethyl)-2-nitrobenzene C7H6ClNO2[2, 3, 61, 64]

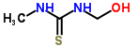
Compound Data

Melting point	**48.75 °C**	**321.90 K**			
CSID	11427	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	0	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	ClCc1ccccc1[N+]([O-])=O				
STD InChIKey	BXCBUWKTXLWPSB-UHFFFAOYAT				

Melting Points

mp °C	source
48.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
49.00	Alfa Aesar
47.00	Oxford University MSDS
51.00	PHYSPROP

1-(hydroxymethyl)-3-methylthiourea C3H8N2OS[9, 48, 64]



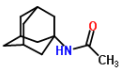
Compound Data

Melting point	**88.33 °C**	**361.48 K**			
CSID	4418329	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	120.1734	**H bond donors**	3	**ACD/LogP**	-1.14
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.22 g/cm^3
SMILES	S=C(NC)NCO				
STD InChIKey	JLMHZVYLAQPMOZ-UHFFFAOYAD				

Melting Points

mp °C	source
88.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
88.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
89.00	PHYSPROP

1-acetamidoadamantane C12H19NO[3, 64]



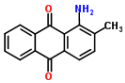
Compound Data

Melting point	**148.25 °C**	**421.40 K**			
CSID	57727	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	193.2854	**H bond donors**	1	**ACD/LogP**	1.83
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	O=C(NC13CC2CC(CC(C1)C2)C3)C				
STD InChIKey	BCVXYGJCDZPKGV-UHFFFAOYAJ				

Melting Points

mp °C	source
148.00	Alfa Aesar
148.50	PHYSPROP

1-amino-2-methyl-anthraquinone C15H11NO2[61, 64]



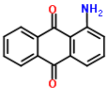
Compound Data

Melting point	**205.25 °C**	**478.40 K**			
CSID	6447	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	237.2533	**H bond donors**	2	**ACD/LogP**	3.81
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	O=C2c1ccccc1C(=O)c3c2ccc(c3N)C				
STD InChIKey	ZLCUIOWQYBYEBG-UHFFFAOYAP				

Melting Points

mp °C	source
205.00	Oxford University MSDS
205.50	PHYSPROP

1-aminoanthraquinone C14H9NO2[3, 61, 64]



Compound Data

Melting point	**252.50 °C**	**525.65 K**			
CSID	6454	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	223.2268	**H bond donors**	2	**ACD/LogP**	3.35
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.38 g/cm^3
SMILES	O=C2c1ccccc1C(=O)c3c2cccc3N				
STD InChIKey	KHUFHLFHOQVFGB-UHFFFAOYAK				

Melting Points

mp °C	source
254.00	Alfa Aesar
250.00	Oxford University MSDS
253.50	PHYSPROP

1-aminonaphthalene C10H9N[2, 2, 64]

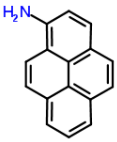
Compound Data

Melting point	**48.73 °C**	**321.88 K**			
CSID	8319	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	2	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	c1cccc2cccc(N)c12				
STD InChIKey	RUFPHBVGCFYCNW-UHFFFAOYAD				

Melting Points

mp °C	source
48.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
49.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
49.20	PHYSPROP

1-aminopyrene C16H11N[3, 35, 61]



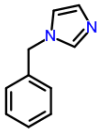
Compound Data

Melting point	**116.67 °C**	**389.82 K**			
CSID	14613	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	217.2652	**H bond donors**	2	**ACD/LogP**	3.89
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	c4cc2ccc1ccc(N)c3c1c2c(cc3)c4				
STD InChIKey	YZVWKHVRBDQPMQ-UHFFFAOYAB				

Melting Points

mp °C	source
118.00	Alfa Aesar
116.00	EPISuite-ChemSpider
116.00	Oxford University MSDS

1-benzylimidazole C10H10N2[3, 64]



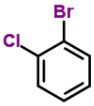
Compound Data

Melting point	**70.00 °C**	**343.15 K**			
CSID	70309	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1998	**H bond donors**	0	**ACD/LogP**	1.46
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	n1ccn(c1)Cc2ccccc2				
STD InChIKey	KKKDZZRICRFGSD-UHFFFAOYAO				

Melting Points

mp °C	source
71.00	Alfa Aesar
69.00	PHYSPROP

1-bromo-2-chlorobenzene C6H4BrCl[3, 64]



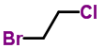
Compound Data

Melting point	**-12.65 °C**	**260.50 K**			
CSID	12230	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	191.453	**H bond donors**	0	**ACD/LogP**	3.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.63 g/cm^3
SMILES	Clc1ccccc1Br				
STD InChIKey	QBELEDRHMPMKHP-UHFFFAOYAF				

Melting Points

mp °C	source
-13.00	Alfa Aesar
-12.30	PHYSPROP

1-bromo-2-chloroethane C2H4BrCl[2, 3, 64]



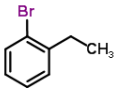
Compound Data

Melting point	**-17.23 °C**	**255.92 K**			
CSID	13854130	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	143.4102	**H bond donors**	0	**ACD/LogP**	1.61
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.67 g/cm^3
SMILES	BrCCCl				
STD InChIKey	IBYHHJPAARCAIE-UHFFFAOYAR				

Melting Points

mp °C	source
-17.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-18.00	Alfa Aesar
-16.70	PHYSPROP

1-bromo-2-ethylbenzene C8H9Br[3, 31, 64]



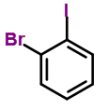
Compound Data

Melting point	**-67.97 °C**	**205.18 K**			
CSID	21111882	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	185.0611	**H bond donors**	0	**ACD/LogP**	3.98
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	CCc1ccccc1Br				
STD InChIKey	HVRUGFJYCAFAAN-UHFFFAOYAK				

Melting Points

mp °C	source
-68.00	Alfa Aesar
-68.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-67.90	PHYSPROP

1-bromo-2-iodobenzene C6H4BrI[2, 3, 64]



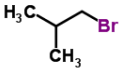
Compound Data

Melting point	**9.83 °C**	**282.98 K**			
CSID	10935	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	282.9044	**H bond donors**	0	**ACD/LogP**	3.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.21 g/cm^3
SMILES	Ic1ccccc1Br				
STD InChIKey	OIRHKGBNGGSCGS-UHFFFAOYAR				

Melting Points

mp °C	source
10.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
10.00	Alfa Aesar
9.50	PHYSPROP

1-bromo-2-methylpropane C4H9Br[3, 31, 64]



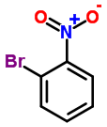
Compound Data

Melting point	**-118.00 °C**	**155.15 K**			
CSID	6307	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	137.0183	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	BrCC(C)C				
STD InChIKey	HLVFKOKELQSXIQ-UHFFFAOYAL				

Melting Points

mp °C	source
-118.00	Alfa Aesar
-117.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-119.00	PHYSPROP

1-bromo-2-nitrobenzene C6H4BrNO2[3, 7, 64]



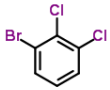
Compound Data

Melting point	**42.67 °C**	**315.82 K**			
CSID	10864	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	202.0055	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.72 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1Br				
STD InChIKey	ORPVVAKYSXQCJI-UHFFFAOYAL				

Melting Points

mp °C	source
42.00	Alfa Aesar
43.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
43.00	PHYSPROP

1-bromo-2,3-dichlorobenzene C6H3BrCl2[3, 64]



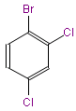
Compound Data

Melting point	**59.00 °C**	**332.15 K**			
CSID	38364	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	225.898	**H bond donors**	0	**ACD/LogP**	3.92
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.74 g/cm^3
SMILES	Clc1cccc(Br)c1Cl				
STD InChIKey	HVKCZUVMQPUWSX-UHFFFAOYAV				

Melting Points

mp °C	source
58.00	Alfa Aesar
60.00	PHYSPROP

1-bromo-2,4-dichlorobenzene C6H3BrCl2[3, 64]



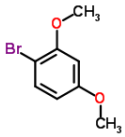
Compound Data

Melting point	**26.50 °C**	**299.65 K**			
CSID	21170125	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	225.898	**H bond donors**	0	**ACD/LogP**	4.04
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.74 g/cm^3
SMILES	Clc1ccc(Br)c(Cl)c1				
STD InChIKey	ISHYFWKKWKXXPL-UHFFFAOYAP				

Melting Points

mp °C	source
27.00	Alfa Aesar
26.00	PHYSPROP

1-bromo-2,4-dimethoxybenzene C8H9BrO2[2, 3]



Compound Data

Melting point	**25.50 °C**	**298.65 K**			
CSID	78722	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	217.0599	**H bond donors**	0	**ACD/LogP**	2.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Brc1ccc(OC)cc1OC				
STD InChIKey	NIUZVSQOXJIHBL-UHFFFAOYAB				

Melting Points

mp °C	source
26.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
25.00	Alfa Aesar

1-bromo-2,4,5-trimethylbenzene C9H11Br[2, 3, 64]

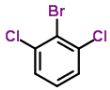
Compound Data

Melting point	**72.00 °C**	**345.15 K**			
CSID	13875161	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	199.0876	**H bond donors**	0	**ACD/LogP**	4.37
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	Cc1cc(C)c(Br)cc1C				
STD InChIKey	SCZXFZRJDVZMJI-UHFFFAOYAP				

Melting Points

mp °C	source
71.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
72.00	Alfa Aesar
73.00	PHYSPROP

1-bromo-2,6-dichlorobenzene C6H3BrCl2[2, 3, 64]



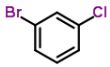
Compound Data

Melting point	**64.00 °C**	**337.15 K**			
CSID	27488	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	225.898	**H bond donors**	0	**ACD/LogP**	4.01
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.74 g/cm^3
SMILES	Clc1cccc(Cl)c1Br				
STD InChIKey	UWOIDOQAQPUVOH-UHFFFAOYAZ				

Melting Points

mp °C	source
66.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
61.00	Alfa Aesar
65.00	PHYSPROP

1-bromo-3-chlorobenzene C6H4BrCl[3, 64]



Compound Data

Melting point	**-21.75 °C**	**251.40 K**			
CSID	13875377	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	191.453	**H bond donors**	0	**ACD/LogP**	3.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.63 g/cm^3
SMILES	Clc1cc(Br)ccc1				
STD InChIKey	JRGGUPZKKTVKOV-UHFFFAOYAS				

Melting Points

mp °C	source
-22.00	Alfa Aesar
-21.50	PHYSPROP

1-bromo-3-chloropropane C3H6BrCl[3, 64]

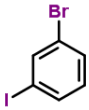
Compound Data

Melting point	**-58.95 °C**	**214.20 K**			
CSID	7715	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	157.4367	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.53 g/cm^3
SMILES	BrCCCCl				
STD InChIKey	MFESCIUQSIBMSM-UHFFFAOYAL				

Melting Points

mp °C	source
-59.00	Alfa Aesar
-58.90	PHYSPROP

1-bromo-3-iodobenzene C6H4BrI[2, 3, 64]



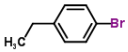
Compound Data

Melting point	**-9.10 °C**	**264.05 K**			
CSID	11073	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	282.9044	**H bond donors**	0	**ACD/LogP**	4.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.21 g/cm^3
SMILES	Ic1cccc(Br)c1				
STD InChIKey	CTPUUDQIXKUAMO-UHFFFAOYAL				

Melting Points

mp °C	source
-9.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-9.00	Alfa Aesar
-9.30	PHYSPROP

1-bromo-4-ethylbenzene C8H9Br[31, 64]



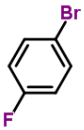
Compound Data

Melting point	**-43.25 °C**	**229.90 K**			
CSID	21106562	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	185.0611	**H bond donors**	0	**ACD/LogP**	3.98
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	CCc1ccc(Br)cc1				
STD InChIKey	URFPRAHGGBYNPW-UHFFFAOYAF				

Melting Points

mp °C	source
-43.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-43.50	PHYSPROP

1-bromo-4-fluorobenzene C_6H_4BrF[3, 64]



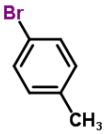
Compound Data

Melting point	**-16.70 °C**	**256.45 K**			
CSID	13875180	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	174.9984	**H bond donors**	0	**ACD/LogP**	2.98
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.59 g/cm^3
SMILES	Fc1ccc(Br)cc1				
STD InChIKey	AITNMTXHTIIIBB-UHFFFAOYAZ				

Melting Points

mp °C	source
-16.00	Alfa Aesar
-17.40	PHYSPROP

1-bromo-4-methylbenzene C_7H_7Br[3, 31, 61, 64]



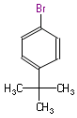
Compound Data

Melting point	**27.50 °C**	**300.65 K**			
CSID	13875258	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	171.0345	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	Cc1ccc(Br)cc1				
STD InChIKey	ZBTMRBYMKUEVEU-UHFFFAOYAF				

Melting Points

mp °C	source
28.00	Alfa Aesar
25.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
28.50	Oxford University MSDS
28.50	PHYSPROP

1-bromo-4-t-butylbenzene $C_{10}H_{13}Br$[2, 3, 64]



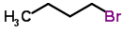
Compound Data

Melting point	**17.00 °C**	**290.15 K**			
CSID	21171393	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	213.1142	**H bond donors**	0	**ACD/LogP**	4.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	CC(C)(C)c1ccc(Br)cc1				
STD InChIKey	XHCAGOVGSDHHNP-UHFFFAOYAL				

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
16.00	Alfa Aesar
19.00	PHYSPROP

1-bromobutane C_4H_9Br[3, 31, 64]



Compound Data

Melting point	**-112.13 °C**	**161.02 K**			
CSID	7711	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	137.0183	**H bond donors**	0	**ACD/LogP**	2.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	BrCCCC				
STD InChIKey	MPPPKRYCTPRNTB-UHFFFAOYAX				

Melting Points

mp °C	source
-112.00	Alfa Aesar
-112.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-112.40	PHYSPROP

1-bromodecane C10H21Br[3, 31, 64]

Compound Data

Melting point	**-29.40 °C**	**243.75 K**			
CSID	7881	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	221.1777	**H bond donors**	0	**ACD/LogP**	5.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	1.07 g/cm^3
SMILES	CCCCCCCCCCBr				
STD InChIKey	MYMSJFSOOQERIO-UHFFFAOYAS				

Melting Points

mp °C	source
-30.00	Alfa Aesar
-29.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-29.20	PHYSPROP

1-bromododecane C12H25Br[3, 31, 64]

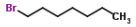
Compound Data

Melting point	**-9.83 °C**	**263.32 K**			
CSID	8579	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	249.2309	**H bond donors**	0	**ACD/LogP**	6.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	1.04 g/cm^3
SMILES	BrCCCCCCCCCCCC				
STD InChIKey	PBLNBZIONSLZBU-UHFFFAOYAT				

Melting Points

mp °C	source
-10.00	Alfa Aesar
-10.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-9.50	PHYSPROP

1-bromoheptane C7H15Br[3, 31, 64]



Compound Data

Melting point	**-57.33 °C**	**215.82 K**			
CSID	11863	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	179.098	**H bond donors**	0	**ACD/LogP**	4.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.14 g/cm^3
SMILES	BrCCCCCCC				
STD InChIKey	LSXKDWGTSHCFPP-UHFFFAOYAD				

Melting Points

mp °C	source
-58.00	Alfa Aesar
-56.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-58.00	PHYSPROP

1-bromohexadecane C16H33Br[3, 64]

Compound Data

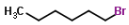
Melting point	**17.50 °C**	**290.65 K**			
CSID	7921	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	305.3372	**H bond donors**	0	**ACD/LogP**	9.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	1.00 g/cm^3
SMILES	BrCCCCCCCCCCCCCCCC				
STD InChIKey	HNTGIJLWHDPAFN-UHFFFAOYAL				

Melting Points

mp °C	source
17.00	Alfa Aesar

18.00	PHYSPROP

1-bromohexane C6H13Br[3, 31, 64]



Compound Data

Melting point	**-84.90 °C**	**188.25 K**			
CSID	7810	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	165.0714	**H bond donors**	0	**ACD/LogP**	3.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.17 g/cm^3
SMILES	BrCCCCCC				
STD InChIKey	MNDIARAMWBIKFW-UHFFFAOYAQ				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-85.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-84.70	PHYSPROP

1-bromonaphthalene C10H7Br[2, 3, 64]

Compound Data

Melting point	**-1.27 °C**	**271.88 K**			
CSID	6735	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	207.0666	**H bond donors**	0	**ACD/LogP**	4.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.48 g/cm^3
SMILES	Brc2cccc1ccccc12				
STD InChIKey	DLKQHBOKULLWDQ-UHFFFAOYAA				

Melting Points

mp °C	source
-1.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-1.00	Alfa Aesar
-1.80	PHYSPROP

1-bromooctadecane C18H37Br[3, 64]

Compound Data

Melting point	**28.10 °C**	**301.25 K**			
CSID	7926	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	333.3904	**H bond donors**	0	**ACD/LogP**	10.18
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	0.98 g/cm^3
SMILES	BrCCCCCCCCCCCCCCCCCC				
STD InChIKey	WSULSMOGMLRGKU-UHFFFAOYAU				

Melting Points

mp °C	source
28.00	Alfa Aesar
28.20	PHYSPROP

1-bromotetradecane C14H29Br[3, 64]

Compound Data

Melting point	**5.30 °C**	**278.45 K**			
CSID	7916	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	277.2841	**H bond donors**	0	**ACD/LogP**	8.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	12	**Predicted density**	1.02 g/cm^3
SMILES	BrCCCCCCCCCCCCCC				
STD InChIKey	KOFZTCSTGIWCQG-UHFFFAOYAB				

Melting Points

mp °C	source
5.00	Alfa Aesar

5.60	PHYSPROP

1-bromoundecane C11H23Br[3, 31, 64]

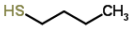
Compound Data

Melting point	**-9.33 °C**	**263.82 K**			
CSID	12221	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	235.2043	**H bond donors**	0	**ACD/LogP**	6.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	1.05 g/cm^3
SMILES	BrCCCCCCCCCCC				
STD InChIKey	IKPSIIAXIDAQLG-UHFFFAOYAT				

Melting Points

mp °C	source
-9.00	Alfa Aesar
-10.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-9.00	PHYSPROP

1-butanethiol C4H10S[3, 4, 61, 64]



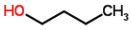
Compound Data

Melting point	**-115.92 °C**	**157.22 K**			
CSID	7721	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	90.1872	**H bond donors**	0	**ACD/LogP**	2.31
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.83 g/cm^3
SMILES	SCCCC				
STD InChIKey	WQAQPCDUOCURKW-UHFFFAOYAG				

Melting Points

mp °C	source
-116.00	Alfa Aesar
-116.00	American Petroleum Institute. Research Project 44; Selected ...
-116.00	Oxford University MSDS
-115.70	PHYSPROP

1-butanol C4H10O[3, 4, 32, 61, 64]



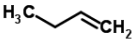
Compound Data

Melting point	**-89.52 °C**	**183.63 K**			
CSID	258	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	74.1216	**H bond donors**	1	**ACD/LogP**	0.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.81 g/cm^3
SMILES	CCCCO				
STD InChIKey	LRHPLDYGYMQRHN-UHFFFAOYAS				

Melting Points

mp °C	source
-90.00	Alfa Aesar
-89.00	American Petroleum Institute. Research Project 44; Selected ...
-89.80	DrugBank
-89.00	Oxford University MSDS
-89.80	PHYSPROP

1-butene C4H8[61, 64, 64, 85]



Compound Data

Melting point	**-185.22 °C**	**87.93 K**			
CSID	7556	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	56.1063	**H bond donors**	0	**ACD/LogP**	2.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.63 g/cm^3
SMILES	CCC=C				

STD InChIKey	VXNZUUAINFGPBY-UHFFFAOYAZ

Melting Points

mp °C	source
-185.00	Oxford University MSDS
-185.30	PHYSPROP
-185.35	Yamamuro O; Matsuo T; Takeda K; Kanaya T; Kawaguchi T; Kaji ...
	Values not used in calculating the average melting point
-145.00	PHYSPROP[1]

1. Value clearly out of range EC

1-butylamine C4H11N[31, 32, 61, 64]

Compound Data

Melting point	**-49.25 °C**	**223.90 K**			
CSID	7716	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	73.1368	**H bond donors**	2	**ACD/LogP**	0.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.74 g/cm^3
SMILES	NCCCC				
STD InChIKey	HQABUPZFAYXKJW-UHFFFAOYAE				

Melting Points

mp °C	source
-49.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-49.00	DrugBank
-49.00	Oxford University MSDS
-50.00	PHYSPROP

1-chloro-1,1-difluoroethane C2H3ClF2[61, 64]

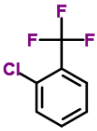
Compound Data

Melting point	**-130.90 °C**	**142.25 K**			
CSID	6148	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.495	**H bond donors**	0	**ACD/LogP**	1.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	ClC(F)(F)C				
STD InChIKey	BHNZEZWIUMJCGF-UHFFFAOYAO				

Melting Points

mp °C	source
-131.00	Oxford University MSDS
-130.80	PHYSPROP

1-chloro-2-(trifluoromethyl)benzene C7H4ClF3[3, 61, 64]



Compound Data

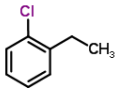
Melting point	**-6.47 °C**	**266.68 K**			
CSID	6655	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	180.5549	**H bond donors**	0	**ACD/LogP**	3.52
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.34 g/cm^3
SMILES	FC(F)(F)c1ccccc1Cl				
STD InChIKey	DGRVQOKCSKDWIH-UHFFFAOYAA				

Melting Points

mp °C	source
-6.00	Alfa Aesar
-7.40	Oxford University MSDS
-6.00	PHYSPROP

1-chloro-2-ethylbenzene C8H9Cl[31, 64]

Compound Data



Melting point	**-82.85 °C**	**190.30 K**			
CSID	21111805	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	140.6101	**H bond donors**	0	**ACD/LogP**	3.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	CCc1ccccc1Cl				
STD InChIKey	CVGAWKYSRYXQOI-UHFFFAOYAS				

Melting Points

mp °C	source
-83.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-82.70	PHYSPROP

1-chloro-2-iodobenzene C6H4ClI[2, 3, 64]

Compound Data

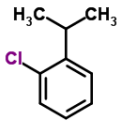
Melting point	**0.90 °C**	**274.05 K**			
CSID	21171406	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	238.4534	**H bond donors**	0	**ACD/LogP**	4.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.93 g/cm^3
SMILES	Ic1ccccc1Cl				
STD InChIKey	MPEOPBCQHNWNFB-UHFFFAOYAL				

Melting Points

mp °C	source
1.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
1.00	Alfa Aesar
0.70	PHYSPROP

1-chloro-2-isopropylbenzene C9H11Cl[31, 64]

Compound Data



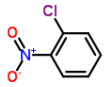
Melting point	**-74.20 °C**	**198.95 K**			
CSID	15532	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	154.6366	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.02 g/cm^3
SMILES	Clc1ccccc1C(C)C				
STD InChIKey	RNEMUWDQJSRDMQ-UHFFFAOYAN				

Melting Points

mp °C	source
-74.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-74.40	PHYSPROP

1-chloro-2-nitrobenzene C6H4ClNO2[2, 3, 61, 64]

Compound Data

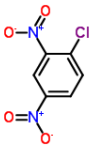


Melting point	**32.88 °C**	**306.02 K**			
CSID	13853953	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	157.5545	**H bond donors**	0	**ACD/LogP**	2.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1Cl				
STD InChIKey	BFCFYVKQTRLZHA-UHFFFAOYAA				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
33.00	Alfa Aesar
32.00	Oxford University MSDS
32.50	PHYSPROP

1-chloro-2,4-dinitrobenzene C6H3ClN2O4[2, 3, 61, 64]



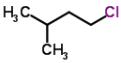
Compound Data

Melting point	**52.25 °C**	**325.40 K**			
CSID	13868426	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	202.552	**H bond donors**	0	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.62 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1Cl)[N+]([O-])=O				
STD InChIKey	VYZAHLCBVHPDDF-UHFFFAOYAS				

Melting Points

mp °C	source
53.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
50.00	Alfa Aesar
53.00	Oxford University MSDS
53.00	PHYSPROP

1-chloro-3-methylbutane C5H11Cl[3, 64]



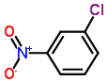
Compound Data

Melting point	**-104.20 °C**	**168.95 K**			
CSID	7605	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.5938	**H bond donors**	0	**ACD/LogP**	2.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.87 g/cm^3
SMILES	ClCCC(C)C				
STD InChIKey	CZHLPWNZCJEPJB-UHFFFAOYAJ				

Melting Points

mp °C	source
-104.00	Alfa Aesar
-104.40	PHYSPROP

1-chloro-3-nitrobenzene C6H4ClNO2[2, 3, 61, 64]



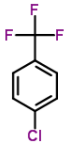
Compound Data

Melting point	**44.75 °C**	**317.90 K**			
CSID	21106013	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	157.5545	**H bond donors**	0	**ACD/LogP**	2.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	O=[N+]([O-])c1cc(Cl)ccc1				
STD InChIKey	KMAQZIILEGKYQZ-UHFFFAOYAS				

Melting Points

mp °C	source
43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
45.00	Alfa Aesar
45.00	Oxford University MSDS
46.00	PHYSPROP

1-chloro-4-(trifluoromethyl)benzene C7H4ClF3[3, 61, 64]



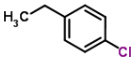
Compound Data

Melting point	**-35.00 °C**	**238.15 K**			
CSID	7116	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	180.5549	**H bond donors**	0	**ACD/LogP**	3.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.34 g/cm^3
SMILES	FC(F)(F)c1ccc(Cl)cc1				
STD InChIKey	QULYNCCPRWKEMF-UHFFFAOYAI				

Melting Points

mp °C	source
-36.00	Alfa Aesar
-36.00	Oxford University MSDS
-33.00	PHYSPROP

1-chloro-4-ethylbenzene C8H9Cl[31, 64]



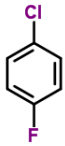
Compound Data

Melting point	**-62.80 °C**	**210.35 K**			
CSID	21242799	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	140.6101	**H bond donors**	0	**ACD/LogP**	3.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	CCc1ccc(Cl)cc1				
STD InChIKey	GPOFSFLJOIAMSA-UHFFFAOYAC				

Melting Points

mp °C	source
-63.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-62.60	PHYSPROP

1-chloro-4-fluorobenzene C6H4ClF[3, 64]



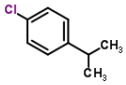
Compound Data

Melting point	**-24.40 °C**	**248.75 K**			
CSID	9228	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	130.5474	**H bond donors**	0	**ACD/LogP**	2.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	Fc1ccc(Cl)cc1				
STD InChIKey	RJCGZNCCVKIBHO-UHFFFAOYAG				

Melting Points

mp °C	source
-22.00	Alfa Aesar
-26.80	PHYSPROP

1-chloro-4-isopropylbenzene C9H11Cl[31, 64]



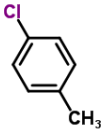
Compound Data

Melting point	**-12.15 °C**	**261.00 K**			
CSID	21159680	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	154.6366	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.02 g/cm^3
SMILES	CC(C)c1ccc(Cl)cc1				
STD InChIKey	FHBSIIZALGOVLM-UHFFFAOYAM				

Melting Points

mp °C	source
-12.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-12.30	PHYSPROP

1-chloro-4-methylbenzene C7H7Cl[2, 3, 61, 64]



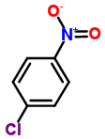
Compound Data

Melting point	**7.50 °C**	**280.65 K**			
CSID	13875160	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	126.5835	**H bond donors**	0	**ACD/LogP**	3.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	Cc1ccc(cc1)Cl				
STD InChIKey	NPDACUSDTOMAMK-UHFFFAOYAI				

Melting Points

mp °C	source
7.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
8.00	Alfa Aesar
7.50	Oxford University MSDS
7.50	PHYSPROP

1-chloro-4-nitrobenzene $C_6H_4ClNO_2$[2, 3, 61, 64]



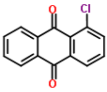
Compound Data

Melting point	**83.77 °C**	**356.92 K**			
CSID	21106020	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	157.5545	**H bond donors**	0	**ACD/LogP**	2.60
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	O=[N+]([O-])c1ccc(Cl)cc1				
STD InChIKey	CZGCEKJOLUNIFY-UHFFFAOYAO				

Melting Points

mp °C	source
84.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
84.00	Alfa Aesar
83.60	Oxford University MSDS
83.50	PHYSPROP

1-chloroanthraquinone $C_{14}H_7ClO_2$[3, 64]



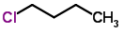
Compound Data

Melting point	**161.50 °C**	**434.65 K**			
CSID	6453	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	242.6572	**H bond donors**	0	**ACD/LogP**	3.98
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	O=C2c1ccccc1C(=O)c3c2cccc3Cl				
STD InChIKey	BOCJQSFSGAZAPQ-UHFFFAOYAU				

Melting Points

mp °C	source
160.00	Alfa Aesar
163.00	PHYSPROP

1-chlorobutane C_4H_9Cl[3, 31, 61, 64]



Compound Data

Melting point	**-123.03 °C**	**150.12 K**			
CSID	7714	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	92.5673	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.87 g/cm^3
SMILES	ClCCCC				
STD InChIKey	VFWCMGCRMGJXDK-UHFFFAOYAR				

Melting Points

mp °C	source
-123.00	Alfa Aesar
-123.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-123.00	Oxford University MSDS
-123.10	PHYSPROP

1-chlorodecane $C_{10}H_{21}Cl$[31, 64]

Compound Data

Melting point	**-31.15 °C**	**242.00 K**			
CSID	13248	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	176.7267	**H bond donors**	0	**ACD/LogP**	5.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.86 g/cm^3
SMILES	ClCCCCCCCCCC				
STD InChIKey	ZTEHOZMYMCEYRM-UHFFFAOYAM				

Melting Points

mp °C	source
-31.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...

-31.30	PHYSPROP

1-chlorododecane C12H25Cl[31, 64]

Compound Data

Melting point	**-9.15 °C**	**264.00 K**			
CSID	7900	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	204.7799	**H bond donors**	0	**ACD/LogP**	6.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	0.86 g/cm^3
SMILES	ClCCCCCCCCCCCC				
STD InChIKey	YAYNEUUHHLGGAH-UHFFFAOYAM				

Melting Points

mp °C	source
-9.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-9.30	PHYSPROP

1-chloroheptane C7H15Cl[31, 64]

Compound Data

Melting point	**-69.75 °C**	**203.40 K**			
CSID	11865	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.647	**H bond donors**	0	**ACD/LogP**	4.16
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.87 g/cm^3
SMILES	ClCCCCCCC				
STD InChIKey	DZMDPHNGKBEVRE-UHFFFAOYAG				

Melting Points

mp °C	source
-70.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-69.50	PHYSPROP

1-chlorononane C9H19Cl[31, 64]

Compound Data

Melting point	**-39.20 °C**	**233.95 K**			
CSID	16268	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	162.7002	**H bond donors**	0	**ACD/LogP**	5.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.86 g/cm^3
SMILES	ClCCCCCCCCC				
STD InChIKey	RKAMCQVGHFRILV-UHFFFAOYAW				

Melting Points

mp °C	source
-39.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-39.40	PHYSPROP

1-chlorooctane C8H17Cl[3, 31, 64]

Compound Data

Melting point	**-57.93 °C**	**215.22 K**			
CSID	7850	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	148.6736	**H bond donors**	0	**ACD/LogP**	4.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.86 g/cm^3
SMILES	ClCCCCCCCC				
STD InChIKey	CNDHHGUSRIZDSL-UHFFFAOYAT				

Melting Points

mp °C	source
-58.00	Alfa Aesar
-58.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-57.80	PHYSPROP

1-chloropropane C3H7Cl[31, 61, 64]

Compound Data

Melting point	**-122.60 °C**	**150.55 K**			
CSID	10437	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	78.5407	**H bond donors**	0	**ACD/LogP**	2.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.88 g/cm^3
SMILES	ClCCC				
STD InChIKey	SNMVRZFUUCLYTO-UHFFFAOYAO				

Melting Points

mp °C	source
-123.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-122.00	Oxford University MSDS
-122.80	PHYSPROP

1-decanol C10H22O[3, 4, 61, 64]

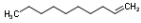
Compound Data

Melting point	**6.72 °C**	**279.88 K**			
CSID	7882	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	158.2811	**H bond donors**	1	**ACD/LogP**	4.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.83 g/cm^3
SMILES	OCCCCCCCCCC				
STD InChIKey	MWKFXSUHUHTGQN-UHFFFAOYAN				

Melting Points

mp °C	source
6.00	Alfa Aesar
7.00	American Petroleum Institute. Research Project 44; Selected ...
7.00	Oxford University MSDS
6.90	PHYSPROP

1-decene C10H20[3, 4, 59, 61, 64, 64]



Compound Data

Melting point	**-66.09 °C**	**207.06 K**			
CSID	12809	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	140.2658	**H bond donors**	0	**ACD/LogP**	5.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.74 g/cm^3
SMILES	CCCCCCCCC=C				
STD InChIKey	AFFLGGQVNFXPEV-UHFFFAOYAO				

Melting Points

mp °C	source
-66.00	Alfa Aesar
-66.00	American Petroleum Institute. Research Project 44; Selected ...
-66.15	NIST Web Book
-66.00	Oxford University MSDS
-66.30	PHYSPROP
	Values not used in calculating the average melting point
-94.00	PHYSPROP[1]

1. Value clearly out of range EC

1-decylamine C10H23N[31, 61, 64]

Compound Data

Melting point	**15.33 °C**	**288.48 K**			
CSID	8576	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	157.2963	**H bond donors**	2	**ACD/LogP**	4.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.80 g/cm^3

SMILES	NCCCCCCCCCCC
STD InChIKey	MHZGKXUYDGKKIU-UHFFFAOYAV

Melting Points

mp °C	source
16.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
13.00	Oxford University MSDS
17.00	PHYSPROP

1-docosanol C22H46O[61, 64]

Compound Data

Melting point	**71.25 °C**	**344.40 K**			
CSID	12100	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	326.6	**H bond donors**	1	**ACD/LogP**	10.44
Phase 25 °C	solid	**Rotatable bonds**	21	**Predicted density**	0.84 g/cm^3
SMILES	OCCCCCCCCCCCCCCCCCCCCCC				
STD InChIKey	NOPFSRXAKWQILS-UHFFFAOYAB				

Melting Points

mp °C	source
70.00	Oxford University MSDS
72.50	PHYSPROP

1-dodecanethiol C12H26S[3, 64]

Compound Data

Melting point	**-7.50 °C**	**265.65 K**			
CSID	7903	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	202.3998	**H bond donors**	0	**ACD/LogP**	6.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.84 g/cm^3
SMILES	CCCCCCCCCCCCS				
STD InChIKey	WNAHIZMDSQCWRP-UHFFFAOYAL				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-8.00	PHYSPROP

1-dodecanol C12H26O[3, 4, 61, 64]

Compound Data

Melting point	**24.50 °C**	**297.65 K**			
CSID	7901	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	186.3342	**H bond donors**	1	**ACD/LogP**	5.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.83 g/cm^3
SMILES	OCCCCCCCCCCCC				
STD InChIKey	LQZZUXJYWNFBMV-UHFFFAOYAU				

Melting Points

mp °C	source
26.00	Alfa Aesar
24.00	American Petroleum Institute. Research Project 44; Selected ...
24.00	Oxford University MSDS
24.00	PHYSPROP

1-dodecene C12H24[3, 4, 61, 64, 64]

Compound Data

Melting point	**-35.48 °C**	**237.67 K**			
CSID	7891	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	168.319	**H bond donors**	0	**ACD/LogP**	6.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.76 g/cm^3
SMILES	CCCCCCCCCCC=C				
STD InChIKey	CRSBERNSMYQZNG-UHFFFAOYAT				

Melting Points

mp °C	source
-37.00	Alfa Aesar
-35.00	American Petroleum Institute. Research Project 44; Selected ...
-35.00	Oxford University MSDS
-35.20	PHYSPROP
-35.20	PHYSPROP

1-eicosanol C20H42O[3, 64]

Compound Data

Melting point	**65.05 °C**	**338.20 K**			
CSID	11898	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	298.5469	**H bond donors**	1	**ACD/LogP**	9.38
Phase 25 °C	solid	**Rotatable bonds**	19	**Predicted density**	0.84 g/cm^3
SMILES	OCCCCCCCCCCCCCCCCCCCC				
STD InChIKey	BTFJIXJJCSYFAL-UHFFFAOYAC				

Melting Points

mp °C	source
64.00	Alfa Aesar
66.10	PHYSPROP

1-eicosene C20H40[4, 64]

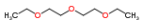
Compound Data

Melting point	**28.75 °C**	**301.90 K**			
CSID	17879	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	280.5316	**H bond donors**	0	**ACD/LogP**	10.87
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.79 g/cm^3
SMILES	C=C\CCCCCCCCCCCCCCCCCC				
STD InChIKey	VAMFXQBUQXONLZ-UHFFFAOYAX				

Melting Points

mp °C	source
29.00	American Petroleum Institute. Research Project 44; Selected ...
28.50	PHYSPROP

1-ethoxy-2-(2-ethoxyethoxy)ethane C8H18O3[3, 61, 64]



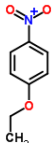
Compound Data

Melting point	**-44.33 °C**	**228.82 K**			
CSID	21106583	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	162.2267	**H bond donors**	0	**ACD/LogP**	0.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.90 g/cm^3
SMILES	CCOCCOCCOCC				
STD InChIKey	RRQYJINTUHWNHW-UHFFFAOYAF				

Melting Points

mp °C	source
-44.00	Alfa Aesar
-44.00	Oxford University MSDS
-45.00	PHYSPROP

1-ethoxy-4-nitrobenzene C8H9NO3[61, 64]



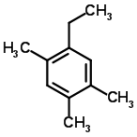
Compound Data

Melting point	**59.00 °C**	**332.15 K**			
CSID	7214	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	167.162	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3
SMILES	[O-][N+](=O)c1ccc(OCC)cc1				
STD InChIKey	NWPKEYHUZKMWKJ-UHFFFAOYAK				

Melting Points

mp °C	source
58.00	Oxford University MSDS
60.00	PHYSPROP

1-ethyl-2,4,5-trimethylbenzene C11H16[4, 64]



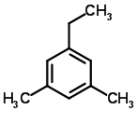
Compound Data

Melting point	**-13.75 °C**	**259.40 K**			
CSID	26801	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	148.2447	**H bond donors**	0	**ACD/LogP**	4.59
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1c(c(cc(c1CC)C)C)C				
STD InChIKey	IYFUQKGDILUVJG-UHFFFAOYAW				

Melting Points

mp °C	source
-14.00	American Petroleum Institute. Research Project 44; Selected ...
-13.50	PHYSPROP

1-ethyl-3,5-dimethylbenzene C10H14[4, 64]



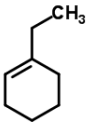
Compound Data

Melting point	**-84.15 °C**	**189.00 K**			
CSID	13038	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1c(cc(cc1CC)C)C				
STD InChIKey	LMAUULKNZLEMGN-UHFFFAOYAP				

Melting Points

mp °C	source
-84.00	American Petroleum Institute. Research Project 44; Selected ...
-84.30	PHYSPROP

1-ethylcyclohexene C8H14[4, 64]



Compound Data

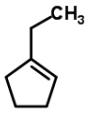
Melting point	**-109.95 °C**	**163.20 K**			
CSID	66568	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	4.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.81 g/cm^3
SMILES	C1(=C/CCCC1)\CC				
STD InChIKey	IFVMAGPISVKRAR-UHFFFAOYAL				

Melting Points

mp °C	source
-110.00	American Petroleum Institute. Research Project 44; Selected ...
-109.90	PHYSPROP

1-ethylcyclopentene C7H12[4, 64]

Compound Data



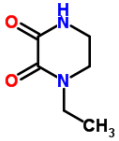
Melting point	**-118.25 °C**	**154.90 K**			
CSID	121113	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.82 g/cm^3
SMILES	C\1=C(/CC)CCC/1				
STD InChIKey	QYYQTLLGVAPKPN-UHFFFAOYAS				

Melting Points

mp °C	source
-118.00	American Petroleum Institute. Research Project 44; Selected ...
-118.50	PHYSPROP

1-ethylpiperazine-2,3-dione C6H10N2O2[3, 64]

Compound Data



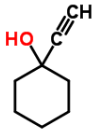
Melting point	**109.00 °C**	**382.15 K**			
CSID	97850	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	142.1558	**H bond donors**	1	**ACD/LogP**	-1.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	O=C1C(=O)N(CC)CCN1				
STD InChIKey	ZBEKOEYCWKIMGU-UHFFFAOYAD				

Melting Points

mp °C	source
110.00	Alfa Aesar
108.00	PHYSPROP

1-ethynyl-1-cyclohexanol C8H12O[2, 3, 64]

Compound Data



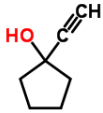
Melting point	**32.17 °C**	**305.32 K**			
CSID	6277	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	124.1803	**H bond donors**	1	**ACD/LogP**	1.73
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.99 g/cm^3
SMILES	C#CC1(O)CCCCC1				
STD InChIKey	QYLFHLNFIHBCPR-UHFFFAOYAD				

Melting Points

mp °C	source
33.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar
31.50	PHYSPROP

1-ethynylcyclopentanol C7H10O[3, 64]

Compound Data



Melting point	**26.00 °C**	**299.15 K**			
CSID	78543	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	110.1537	**H bond donors**	1	**ACD/LogP**	1.17
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	C#CC1(O)CCCC1				
STD InChIKey	LQMDOONLLAJAPZ-UHFFFAOYAX				

Melting Points

mp °C	source
25.00	Alfa Aesar
27.00	PHYSPROP

1-fluoro-2-iodobenzene C6H4FI[3, 64]

Compound Data

Melting point	**-41.75 °C**	**231.40 K**

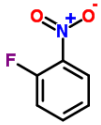
CSID	21168731	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	221.9988	**H bond donors**	0	**ACD/LogP**	3.21
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.92 g/cm^3
SMILES	Fc1ccccc1I				
STD InChIKey	TYHUGKGZNOULKD-UHFFFAOYAT				

Melting Points

mp °C	source
-42.00	Alfa Aesar
-41.50	PHYSPROP

1-fluoro-2-nitrobenzene C6H4FNO2[3, 64]

Compound Data



Melting point	**-7.00 °C**	**266.15 K**			
CSID	66528	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	141.0999	**H bond donors**	0	**ACD/LogP**	1.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1F				
STD InChIKey	PWKNBLFSJAVFAB-UHFFFAOYAW				

Melting Points

mp °C	source
-8.00	Alfa Aesar
-6.00	PHYSPROP

1-fluoro-2,4-dinitrobenzene C6H3FN2O4[3, 61, 64]

Compound Data

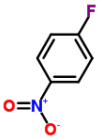
Melting point	**26.60 °C**	**299.75 K**			
CSID	21106037	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	186.0974	**H bond donors**	0	**ACD/LogP**	1.16
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.59 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1F)[N+]([O-])=O				
STD InChIKey	LOTKRQAVGJMPNV-UHFFFAOYAZ				

Melting Points

mp °C	source
27.00	Alfa Aesar
27.00	Oxford University MSDS
25.80	PHYSPROP

1-fluoro-4-nitrobenzene C6H4FNO2[3, 61, 64]

Compound Data



Melting point	**21.67 °C**	**294.82 K**			
CSID	13856885	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	141.0999	**H bond donors**	0	**ACD/LogP**	1.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	O=[N+]([O-])c1ccc(F)cc1				
STD InChIKey	WFQDTOYDVUWQMS-UHFFFAOYAC				

Melting Points

mp °C	source
23.00	Alfa Aesar
21.00	Oxford University MSDS
21.00	PHYSPROP

1-fluoronaphthalene C10H7F[3, 61, 64]

Compound Data

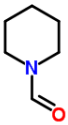
Melting point	**-10.67 °C**	**262.48 K**			
CSID	9078	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	146.161	**H bond donors**	0	**ACD/LogP**	3.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	Fc2cccc1ccccc12				
STD InChIKey	CWLKTJOTWITYSI-UHFFFAOYAY				

Melting Points

mp °C	source
-10.00	Alfa Aesar
-13.00	Oxford University MSDS
-9.00	PHYSPROP

1-formylpiperidine C6H11NO[3, 64]

Compound Data



Melting point	**-30.90 °C**	**242.25 K**			
CSID	16486	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	113.1576	**H bond donors**	0	**ACD/LogP**	0.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.09 g/cm^3
SMILES	O=CN1CCCCC1				
STD InChIKey	FEWLNYSYJNLUOO-UHFFFAOYAJ				

Melting Points

mp °C	source
-31.00	Alfa Aesar
-30.80	PHYSPROP

1-heptadecanol C17H36O[2, 3, 61, 64]

Compound Data

Melting point	**55.70 °C**	**328.85 K**			
CSID	14348	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	256.4671	**H bond donors**	1	**ACD/LogP**	7.78
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	0.84 g/cm^3
SMILES	OCCCCCCCCCCCCCCCCC				
STD InChIKey	GOQYKNQRPGWPLP-UHFFFAOYAD				

Melting Points

mp °C	source
58.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
57.00	Oxford University MSDS
53.80	PHYSPROP

1-heptadecene C17H34[4, 64]

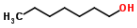
Compound Data

Melting point	**11.25 °C**	**284.40 K**			
CSID	21723	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	238.4519	**H bond donors**	0	**ACD/LogP**	9.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	0.78 g/cm^3
SMILES	C(=C)\CCCCCCCCCCCCCCC				
STD InChIKey	ADOBXTDBFNCOBN-UHFFFAOYAF				

Melting Points

mp °C	source
11.00	American Petroleum Institute. Research Project 44; Selected ...
11.50	PHYSPROP

1-heptanol C7H16O[3, 4, 28, 61, 64]



Compound Data

Melting point	**-34.24 °C**	**238.91 K**			
CSID	7837	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	116.2013	**H bond donors**	1	**ACD/LogP**	2.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.82 g/cm^3
SMILES	OCCCCCCC				
STD InChIKey	BBMCTIGTTCKYKF-UHFFFAOYAV				

Melting Points

mp °C	source
-34.00	Alfa Aesar
-34.00	American Petroleum Institute. Research Project 44; Selected ...
-33.20	CRC Handbook of Chemistry and Physics
-36.00	Oxford University MSDS
-34.00	PHYSPROP

1-heptene C7H14[3, 4, 59, 64]

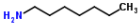
Compound Data

Melting point	**-119.46 °C**	**153.69 K**			
CSID	11121	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.70 g/cm^3
SMILES	C=C\CCCCC				
STD InChIKey	ZGEGCLOFRBLKSE-UHFFFAOYAB				

Melting Points

mp °C	source
-119.00	Alfa Aesar
-119.00	American Petroleum Institute. Research Project 44; Selected ...
-120.15	NIST Web Book
-119.70	PHYSPROP

1-heptylamine C7H17N[3, 31, 64]



Compound Data

Melting point	**-19.67 °C**	**253.48 K**			
CSID	7835	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	115.2166	**H bond donors**	2	**ACD/LogP**	2.52
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.78 g/cm^3
SMILES	NCCCCCCC				
STD InChIKey	WJYIASZWHGOTOU-UHFFFAOYAD				

Melting Points

mp °C	source
-23.00	Alfa Aesar
-18.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-18.00	PHYSPROP

1-hexadecanethiol C16H34S[3, 64]

Compound Data

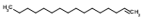
Melting point	**20.00 °C**	**293.15 K**			
CSID	17019	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	258.5062	**H bond donors**	0	**ACD/LogP**	8.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	15	**Predicted density**	0.84 g/cm^3
SMILES	SCCCCCCCCCCCCCCCC				
STD InChIKey	ORTRWBYBJVGVQC-UHFFFAOYAT				

Melting Points

mp °C	source
21.00	Alfa Aesar

19.00	PHYSPROP

1-hexadecene C16H32[3, 4, 64]



Compound Data

Melting point	**4.03 °C**	**277.18 K**			
CSID	11889	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	224.4253	**H bond donors**	0	**ACD/LogP**	8.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	13	**Predicted density**	0.78 g/cm^3
SMILES	C=C\CCCCCCCCCCCCCC				
STD InChIKey	GQEZCXVZFLOKMC-UHFFFAOYAH				

Melting Points

mp °C	source
4.00	Alfa Aesar
4.00	American Petroleum Institute. Research Project 44; Selected ...
4.10	PHYSPROP

1-hexanethiol C6H14S[3, 4, 64]

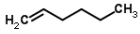
Compound Data

Melting point	**-80.67 °C**	**192.48 K**			
CSID	7815	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.2404	**H bond donors**	0	**ACD/LogP**	3.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.83 g/cm^3
SMILES	SCCCCCC				
STD InChIKey	PMBXCGGQNSVESQ-UHFFFAOYAC				

Melting Points

mp °C	source
-81.00	Alfa Aesar
-80.00	American Petroleum Institute. Research Project 44; Selected ...
-81.00	PHYSPROP

1-hexene C6H12[3, 4, 59, 61, 64]



Compound Data

Melting point	**-139.97 °C**	**133.18 K**			
CSID	11109	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.36
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.69 g/cm^3
SMILES	CCCCC=C				
STD InChIKey	LIKMAJRDDDTEIG-UHFFFAOYAY				

Melting Points

mp °C	source
-140.00	Alfa Aesar
-140.00	American Petroleum Institute. Research Project 44; Selected ...
-140.15	NIST Web Book
-140.00	Oxford University MSDS
-139.70	PHYSPROP

1-hexylamine C6H15N[3, 31, 61, 64]

Compound Data

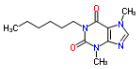
Melting point	**-21.98 °C**	**251.17 K**			
CSID	7811	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	101.19	**H bond donors**	2	**ACD/LogP**	2.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.77 g/cm^3
SMILES	CCCCCCN				
STD InChIKey	BMVXCPBXGZKUPN-UHFFFAOYAQ				

Melting Points

mp °C	source
-19.00	Alfa Aesar
-23.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-23.00	Oxford University MSDS
-22.90	PHYSPROP

1-hexyltheobromine C13H20N4O2[3, 64]

Compound Data



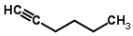
Melting point	**81.75 °C**	**354.90 K**			
CSID	63738	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	264.3235	**H bond donors**	0	**ACD/LogP**	2.53
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.23 g/cm^3
SMILES	O=C2N(c1ncn(c1C(=O)N2CCCCCC)C)C				
STD InChIKey	MRWQRJMESRRJJB-UHFFFAOYAV				

Melting Points

mp °C	source
81.00	Alfa Aesar
82.50	PHYSPROP

1-hexyne C6H10[3, 4, 64]

Compound Data



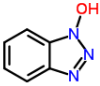
Melting point	**-131.97 °C**	**141.18 K**			
CSID	12209	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.70
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.74 g/cm^3
SMILES	CCCCC#C				
STD InChIKey	CGHIBGNXEGJPQZ-UHFFFAOYAY				

Melting Points

mp °C	source
-132.00	Alfa Aesar
-132.00	American Petroleum Institute. Research Project 44; Selected ...
-131.90	PHYSPROP

1-hydroxybenzotriazole C6H5N3O[61, 64]

Compound Data



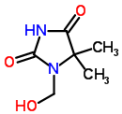
Melting point	**158.25 °C**	**431.40 K**			
CSID	68282	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	135.1234	**H bond donors**	1	**ACD/LogP**	0.69
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.51 g/cm^3
SMILES	n1nn(O)c2ccccc12				
STD InChIKey	ASOKPJOREAFHNY-UHFFFAOYAP				

Melting Points

mp °C	source
159.00	Oxford University MSDS
157.50	PHYSPROP

1-hydroxymethyl-5,5-dimethylhydantoin C6H10N2O3[3, 64]

Compound Data



Melting point	**102.50 °C**	**375.65 K**			
CSID	60357	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	158.1552	**H bond donors**	2	**ACD/LogP**	-0.92
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.26 g/cm^3
SMILES	O=C1NC(=O)N(CO)C1(C)C				

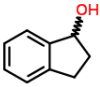
STD InChIKey	SIQZJFKTROUNPI-UHFFFAOYAW

Melting Points

mp °C	source
105.00	Alfa Aesar
100.00	PHYSPROP

1-indanol C9H10O[3, 64]

Compound Data



Melting point	**53.40 °C**	**326.55 K**			
CSID	21394	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	134.1751	**H bond donors**	1	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	OC2c1ccccc1CC2				
STD InChIKey	YIAPLDFPUUJILH-UHFFFAOYAX				

Melting Points

mp °C	source
52.00	Alfa Aesar
54.80	PHYSPROP

1-indanone C9H8O[3, 64]

Compound Data

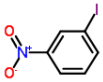
Melting point	**41.00 °C**	**314.15 K**			
CSID	6479	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	132.1592	**H bond donors**	0	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.15 g/cm^3
SMILES	O=C2c1ccccc1CC2				
STD InChIKey	QNXSIUBBGPHDDE-UHFFFAOYAP				

Melting Points

mp °C	source
40.00	Alfa Aesar
42.00	PHYSPROP

1-iodo-3-nitrobenzene C6H4INO2[2, 3, 61, 64]

Compound Data



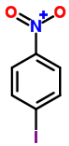
Melting point	**37.62 °C**	**310.77 K**			
CSID	21106127	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	249.0059	**H bond donors**	0	**ACD/LogP**	2.94
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.02 g/cm^3
SMILES	O=[N+]([O-])c1cc(I)ccc1				
STD InChIKey	CBYAZOKPJYBCHE-UHFFFAOYAB				

Melting Points

mp °C	source
38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
37.00	Alfa Aesar
37.00	Oxford University MSDS
38.50	PHYSPROP

1-iodo-4-nitrobenzene C6H4INO2[2, 3, 61, 64]

Compound Data



Melting point	**174.68 °C**	**447.82 K**			
CSID	11982	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	249.0059	**H bond donors**	0	**ACD/LogP**	2.97
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.02 g/cm^3
SMILES	O=[N+]([O-])c1ccc(I)cc1				

STD InChIKey	SCCCFNJTCDSLCY-UHFFFAOYAN

Melting Points

mp °C	source
173.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
175.00	Alfa Aesar
176.00	Oxford University MSDS
174.70	PHYSPROP

1-iododecane C10H21I[3, 31, 64]

Compound Data

Melting point	**-16.10 °C**	**257.05 K**			
CSID	15480	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	268.1782	**H bond donors**	0	**ACD/LogP**	6.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	1.26 g/cm^3
SMILES	ICCCCCCCCCC				
STD InChIKey	SKIDNYUZJPMKFC-UHFFFAOYAR				

Melting Points

mp °C	source
-16.00	Alfa Aesar
-16.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-16.30	PHYSPROP

1-iodododecane C12H25I[3, 31, 64]

Compound Data

Melting point	**-0.90 °C**	**272.25 K**			
CSID	19108	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	296.2314	**H bond donors**	0	**ACD/LogP**	7.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	1.21 g/cm^3
SMILES	ICCCCCCCCCCCC				
STD InChIKey	GCDPERPXPREHJF-UHFFFAOYAV				

Melting Points

mp °C	source
-3.00	Alfa Aesar
0.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
0.30	PHYSPROP

1-iodoheptane C7H15I[3, 31, 64]

Compound Data

Melting point	**-48.07 °C**	**225.08 K**			
CSID	19100	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	226.0985	**H bond donors**	0	**ACD/LogP**	4.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.39 g/cm^3
SMILES	ICCCCCCC				
STD InChIKey	LMHCYRULPLGEEZ-UHFFFAOYAO				

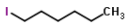
Melting Points

mp °C	source
-48.00	Alfa Aesar
-48.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-48.20	PHYSPROP

1-iodohexane C6H13I[3, 31, 64]

Compound Data

Melting point	**-74.73 °C**	**198.42 K**			
CSID	12010	**H bond acceptors**	0	**Rule of 5 violations**	0



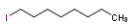
Molecular weight	212.0719	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.45 g/cm^3
SMILES	ICCCCCC				
STD InChIKey	ANOOTOPTCJRUPK-UHFFFAOYAW				

Melting Points

mp °C	source
-75.00	Alfa Aesar
-75.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-74.20	PHYSPROP

1-iodooctane C8H17I[3, 31, 64]

Compound Data



Melting point	**-45.23 °C**	**227.92 K**			
CSID	11874	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	240.125	**H bond donors**	0	**ACD/LogP**	5.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	1.34 g/cm^3
SMILES	ICCCCCCCC				
STD InChIKey	UWLHSHAHTBJTBA-UHFFFAOYAQ				

Melting Points

mp °C	source
-46.00	Alfa Aesar
-44.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-45.70	PHYSPROP

1-iodopentane C5H11I[3, 31, 64]

Compound Data

Melting point	**-85.87 °C**	**187.28 K**			
CSID	11830	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	198.0453	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.52 g/cm^3
SMILES	ICCCCC				
STD InChIKey	BLXSFCHWMBESKV-UHFFFAOYAK				

Melting Points

mp °C	source
-86.00	Alfa Aesar
-86.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-85.60	PHYSPROP

1-iodopropane C3H7I[3, 31, 61, 64]

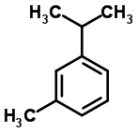
Compound Data

Melting point	**-101.08 °C**	**172.07 K**			
CSID	31029	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	169.9921	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.75 g/cm^3
SMILES	ICCC				
STD InChIKey	PVWOIHVRPOBWPI-UHFFFAOYAJ				

Melting Points

mp °C	source
-101.00	Alfa Aesar
-101.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-101.00	Oxford University MSDS
-101.30	PHYSPROP

1-isopropyl-3-methylbenzene C10H14[4, 64]



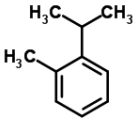
Compound Data

Melting point	**-63.85 °C**	**209.30 K**			
CSID	10355	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.86 g/cm^3
SMILES	c1ccc(cc1C(C)C)C				
STD InChIKey	XCYJPXQACVEIOS-UHFFFAOYAE				

Melting Points

mp °C	source
-64.00	American Petroleum Institute. Research Project 44; Selected ...
-63.70	PHYSPROP

1-isopropyl-3-methylbenzene C10H14[4, 64]



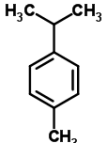
Compound Data

Melting point	**-71.75 °C**	**201.40 K**			
CSID	10253	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.86 g/cm^3
SMILES	c1cccc(c1C(C)C)C				
STD InChIKey	WWRCMNKATXZARA-UHFFFAOYAL				

Melting Points

mp °C	source
-72.00	American Petroleum Institute. Research Project 44; Selected ...
-71.50	PHYSPROP

1-isopropyl-4-methylbenzene C10H14[3, 4, 61, 64, 64]



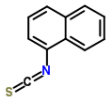
Compound Data

Melting point	**-68.18 °C**	**204.97 K**			
CSID	7183	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.86 g/cm^3
SMILES	c1cc(ccc1C(C)C)C				
STD InChIKey	HFPZCAJZSCWRBC-UHFFFAOYAD				

Melting Points

mp °C	source
-68.00	Alfa Aesar
-68.00	American Petroleum Institute. Research Project 44; Selected ...
-68.00	Oxford University MSDS
-68.90	PHYSPROP
-68.00	PHYSPROP

1-isothiocyanatonaphthalene C11H7NS[3, 61, 64]



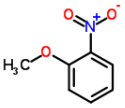
Compound Data

Melting point	**57.33 °C**	**330.48 K**			
CSID	10609	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	185.245	**H bond donors**	0	**ACD/LogP**	4.47
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	S=C=N/c2cccc1ccccc12				
STD InChIKey	JBDOSUUXMYMWQH-UHFFFAOYAA				

Melting Points

mp °C	source
56.00	Alfa Aesar
58.00	Oxford University MSDS
58.00	PHYSPROP

1-methoxy-2-nitrobenzene C7H7NO3[2, 3, 61, 64]



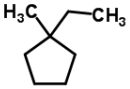
Compound Data

Melting point	**9.97 °C**	**283.12 K**			
CSID	6781	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	153.1354	**H bond donors**	0	**ACD/LogP**	1.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.22 g/cm^3
SMILES	[O-][N+](=O)c1ccccc1OC				
STD InChIKey	CFBYEGUGFPZCNF-UHFFFAOYAE				

Melting Points

mp °C	source
10.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
10.00	Alfa Aesar
9.40	Oxford University MSDS
10.50	PHYSPROP

1-methyl-1-ethylcyclopentane C8H16[4, 64]



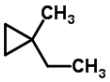
Compound Data

Melting point	**-143.90 °C**	**129.25 K**			
CSID	26072	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.78 g/cm^3
SMILES	CC1(CC)CCCC1				
STD InChIKey	LETYIFNDQBJGPJ-UHFFFAOYAU				

Melting Points

mp °C	source
-144.00	American Petroleum Institute. Research Project 44; Selected ...
-143.80	PHYSPROP

1-methyl-1-ethylcyclopropane C6H12[4, 64]



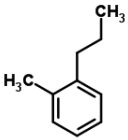
Compound Data

Melting point	**-130.10 °C**	**143.05 K**			
CSID	84221	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.77 g/cm^3
SMILES	CC1(CC)CC1				
STD InChIKey	CXYUCHDVLWUDNS-UHFFFAOYAK				

Melting Points

mp °C	source
-130.00	American Petroleum Institute. Research Project 44; Selected ...
-130.20	PHYSPROP

1-methyl-2-propylbenzene C10H14[4, 64]



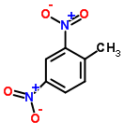
Compound Data

Melting point	**-60.15 °C**	**213.00 K**			
CSID	13471	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.86 g/cm^3
SMILES	c1cccc(c1CCC)C				
STD InChIKey	YQZBFMJOASEONC-UHFFFAOYAW				

Melting Points

mp °C	source
-60.00	American Petroleum Institute. Research Project 44; Selected ...
-60.30	PHYSPROP

1-methyl-2,4-dinitrobenzene C7H6N2O4[2, 3, 61, 64]



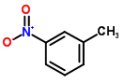
Compound Data

Melting point	**69.38 °C**	**342.52 K**			
CSID	8150	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	182.1335	**H bond donors**	0	**ACD/LogP**	2.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Cc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	RMBFBMJGBANMMK-UHFFFAOYAC				

Melting Points

mp °C	source
69.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
69.00	Alfa Aesar
68.50	Oxford University MSDS
71.00	PHYSPROP

1-methyl-3-nitrobenzene C7H7NO2[2, 3, 61, 64]



Compound Data

Melting point	**15.75 °C**	**288.90 K**			
CSID	21106146	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	0	**ACD/LogP**	2.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	O=[N+]([O-])c1cccc(C)c1				
STD InChIKey	QZYHIOPPLUPUJF-UHFFFAOYAJ				

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
16.00	Alfa Aesar
15.50	Oxford University MSDS
15.50	PHYSPROP

1-methyl-4-nitrobenzene C7H7NO2[2, 3, 61, 64, 72]

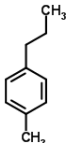
Compound Data

Melting point	**52.32 °C**	**325.47 K**			
CSID	13863774	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	0	**ACD/LogP**	2.41
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C)cc1				
STD InChIKey	ZPTVNYMJQHSSEA-UHFFFAOYAU				

Melting Points

mp °C	source
54.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
52.00	Alfa Aesar
51.00	Oxford University MSDS
51.60	PHYSPROP
53.00	Sigma-Aldrich

1-methyl-4-propylbenzene C10H14[4, 64]



Compound Data

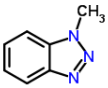
Melting point	**-63.80 °C**	**209.35 K**			
CSID	13473	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.86 g/cm^3
SMILES	c1cc(ccc1CCC)C				
STD InChIKey	JXFVMNFKABWTHD-UHFFFAOYAL				

Melting Points

mp °C	source
-64.00	American Petroleum Institute. Research Project 44; Selected ...
-63.60	PHYSPROP

1-methylbenzotriazole C7H7N3[3, 64]

Compound Data



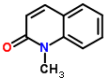
Melting point	**64.75 °C**	**337.90 K**			
CSID	24133	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	133.1506	**H bond donors**	0	**ACD/LogP**	1.06
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	n1nn(c2ccccc12)C				
STD InChIKey	HXQHRUJXQJEGER-UHFFFAOYAL				

Melting Points

mp °C	source
65.00	Alfa Aesar
64.50	PHYSPROP

1-methylcarbostyril C10H9NO[3, 64]

Compound Data



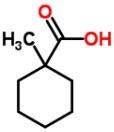
Melting point	**74.50 °C**	**347.65 K**			
CSID	11327	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	159.1846	**H bond donors**	0	**ACD/LogP**	1.55
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	O=C2/C=C\c1c(cccc1)N2C				
STD InChIKey	QYEMNJMSULGQRD-UHFFFAOYAE				

Melting Points

mp °C	source
75.00	Alfa Aesar
74.00	PHYSPROP

1-methylcyclohexanecarboxylic acid C8H14O2[3, 48, 64]

Compound Data



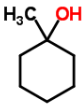
Melting point	**37.83 °C**	**310.98 K**			
CSID	63909	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	142.1956	**H bond donors**	1	**ACD/LogP**	2.31
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	O=C(O)C1(C)CCCCC1				
STD InChIKey	REHQLKUNRPCYEW-UHFFFAOYAN				

Melting Points

mp °C	source
38.00	Alfa Aesar
38.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
37.50	PHYSPROP

1-methylcyclohexanol C7H14O[2, 3, 64]

Compound Data



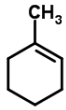
Melting point	**25.67 °C**	**298.82 K**			
CSID	11063	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	114.1855	**H bond donors**	1	**ACD/LogP**	1.66
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.94 g/cm^3
SMILES	CC1(CCCCC1)O				
STD InChIKey	VTBOTOBFGSVRMA-UHFFFAOYAF				

Melting Points

mp °C	source
26.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
26.00	Alfa Aesar
25.00	PHYSPROP

1-methylcyclohexene C7H12[4, 59, 61, 64]

Compound Data



Melting point	**-120.28 °C**	**152.87 K**			
CSID	11086	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	3.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.82 g/cm^3
SMILES	CC1=CCCCC1				
STD InChIKey	CTMHWPIWNRWQEG-UHFFFAOYAY				

Melting Points

mp °C	source
-120.00	American Petroleum Institute. Research Project 44; Selected ...
-120.45	NIST Web Book
-120.40	PHYSPROP
	Values not used in calculating the average melting point
0.00	Oxford University MSDS[1]

1. clearly out of range JCB

1-methylcyclopentanol C6H12O[2, 3, 64]

Compound Data

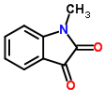
Melting point	**36.67 °C**	**309.82 K**			
CSID	66464	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	100.1589	**H bond donors**	1	**ACD/LogP**	1.32
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.96 g/cm^3
SMILES	OC1(C)CCCC1				
STD InChIKey	CAKWRXVKWGUISE-UHFFFAOYAG				

Melting Points

mp °C	source
37.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
37.00	Alfa Aesar
36.00	PHYSPROP

1-methylisatin C9H7NO2[3, 64]

Compound Data



Melting point	**131.25 °C**	**404.40 K**			
CSID	15517	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	161.1574	**H bond donors**	0	**ACD/LogP**	0.58
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.31 g/cm^3
SMILES	O=C2c1ccccc1N(C2=O)C				
STD InChIKey	VCYBVWFTGAZHGH-UHFFFAOYAR				

Melting Points

mp °C	source
131.00	Alfa Aesar
131.50	PHYSPROP

1-methylpyrrolidin-2-one C5H9NO[3, 61, 64]

Compound Data

Melting point	**-23.67 °C**	**249.48 K**			
CSID	12814	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	99.1311	**H bond donors**	0	**ACD/LogP**	0.00

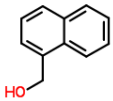
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.03 g/cm
SMILES	CN1CCCC1=O				
STD InChIKey	SECXISVLQFMRJM-UHFFFAOYAL				

Melting Points

mp °C	source
-24.00	Alfa Aesar
-23.00	Oxford University MSDS
-24.00	PHYSPROP

1-naphthalenemethanol C11H10O[3, 64]

Compound Data



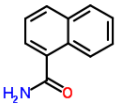
Melting point	**62.50 °C**	**335.65 K**			
CSID	19669	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	158.1965	**H bond donors**	1	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	OCc2cccc1ccccc12				
STD InChIKey	PBLNHHSDYFYZNC-UHFFFAOYAF				

Melting Points

mp °C	source
61.00	Alfa Aesar
64.00	PHYSPROP

1-naphthamide C11H9NO[3, 64]

Compound Data



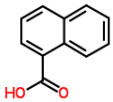
Melting point	**206.90 °C**	**480.05 K**			
CSID	67788	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	171.1953	**H bond donors**	2	**ACD/LogP**	1.97
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.20 g/cm^3
SMILES	O=C(N)c2cccc1ccccc12				
STD InChIKey	RMHJJUOPOWPRBP-UHFFFAOYAG				

Melting Points

mp °C	source
208.00	Alfa Aesar
205.80	PHYSPROP

1-naphthoic acid C11H8O2[3, 61, 64]

Compound Data



Melting point	**161.33 °C**	**434.48 K**			
CSID	6586	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.18	**H bond donors**	1	**ACD/LogP**	3.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	O=C(O)c2cccc1ccccc12				
STD InChIKey	LNETULKMXZVUST-UHFFFAOYAH				

Melting Points

mp °C	source
161.00	Alfa Aesar
162.00	Oxford University MSDS
161.00	PHYSPROP

1-naphthol C10H8O[2, 3, 61, 64]

Compound Data

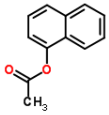
Melting point	**95.50 °C**	**368.65 K**			
CSID	6739	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	144.1699	**H bond donors**	1	**ACD/LogP**	2.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Oc2cccc1ccccc12				
STD InChIKey	KJCVRFUGPWSIIH-UHFFFAOYAZ				

Melting Points

mp °C	source
96.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
96.00	Alfa Aesar
95.00	Oxford University MSDS
95.00	PHYSPROP

1-naphthyl acetate C12H10O2[3, 64]

Compound Data



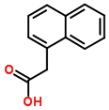
Melting point	**44.75 °C**	**317.90 K**			
CSID	12691	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	0	**ACD/LogP**	2.79
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.16 g/cm^3
SMILES	O=C(Oc2cccc1ccccc12)C				
STD InChIKey	VGKONPUVOVVNSU-UHFFFAOYAE				

Melting Points

mp °C	source
45.00	Alfa Aesar
44.50	PHYSPROP

1-naphthylacetic acid C12H10O2[3, 32, 64]

Compound Data



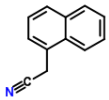
Melting point	**133.33 °C**	**406.48 K**			
CSID	6601	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	1	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C(O)Cc2cccc1ccccc12				
STD InChIKey	PRPINYUDVPFIRX-UHFFFAOYAF				

Melting Points

mp °C	source
130.00	Alfa Aesar
135.00	DrugBank
135.00	PHYSPROP

1-naphthylacetonitrile C12H9N[3, 64]

Compound Data

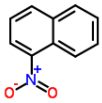


Melting point	**33.25 °C**	**306.40 K**			
CSID	8277	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	167.2066	**H bond donors**	0	**ACD/LogP**	2.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	N#CCc2cccc1ccccc12				
STD InChIKey	OQRMWUNUKVUHQO-UHFFFAOYAB				

Melting Points

mp °C	source
34.00	Alfa Aesar
32.50	PHYSPROP

1-nitronaphthalene C10H7NO2[3, 61, 64]



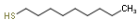
Compound Data

Melting point	**59.83 °C**	**332.98 K**			
CSID	6588	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	173.1681	**H bond donors**	0	**ACD/LogP**	3.18
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.28 g/cm^3
SMILES	[O-][N+](=O)c2cccc1ccccc12				
STD InChIKey	RJKGJBPXVHTNJL-UHFFFAOYAZ				

Melting Points

mp °C	source
57.00	Alfa Aesar
61.50	Oxford University MSDS
61.00	PHYSPROP

1-nonanethiol C9H20S[4, 64]



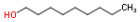
Compound Data

Melting point	**-20.05 °C**	**253.10 K**			
CSID	14349	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	160.3201	**H bond donors**	0	**ACD/LogP**	5.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.84 g/cm^3
SMILES	CCCCCCCCCS				
STD InChIKey	ZVEZMVFBMOOHAT-UHFFFAOYAL				

Melting Points

mp °C	source
-20.00	American Petroleum Institute. Research Project 44; Selected ...
-20.10	PHYSPROP

1-nonanol C9H20O[3, 4, 61, 64, 86]



Compound Data

Melting point	**-5.60 °C**	**267.55 K**			
CSID	8574	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	144.2545	**H bond donors**	1	**ACD/LogP**	3.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.83 g/cm^3
SMILES	CCCCCCCCCO				
STD InChIKey	ZWRUINPWMLAQRD-UHFFFAOYAC				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-5.00	American Petroleum Institute. Research Project 44; Selected ...
-7.00	Oxford University MSDS
-5.00	PHYSPROP
-4.00	Zenitech

1-nonene C9H18[4, 59, 64]

Compound Data

Melting point	**-81.82 °C**	**191.33 K**			
CSID	29025	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	126.2392	**H bond donors**	0	**ACD/LogP**	5.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.73 g/cm^3
SMILES	C=C\CCCCCCC				
STD InChIKey	JRZJOMJEPLMPRA-UHFFFAOYAK				

Melting Points

mp °C	source
-81.00	American Petroleum Institute. Research Project 44; Selected ...
-83.15	NIST Web Book
-81.30	PHYSPROP

1-octadecanethiol C18H38S[3, 64]

Compound Data

Melting point	**31.00 °C**	**304.15 K**			
CSID	16913	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	286.5593	**H bond donors**	0	**ACD/LogP**	9.59
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.84 g/cm^3
SMILES	CCCCCCCCCCCCCCCCCCCS				
STD InChIKey	QJAOYSPHSNGHNC-UHFFFAOYAP				

Melting Points

mp °C	source
32.00	Alfa Aesar
30.00	PHYSPROP

1-octadecanol C18H38O[2, 3, 64]

Compound Data

Melting point	**59.50 °C**	**332.65 K**			
CSID	7928	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	270.4937	**H bond donors**	1	**ACD/LogP**	8.31
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.84 g/cm^3
SMILES	OCCCCCCCCCCCCCCCCCCC				
STD InChIKey	GLDOVTGHNKAZLK-UHFFFAOYAZ				

Melting Points

mp °C	source
61.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
58.00	Alfa Aesar
59.50	PHYSPROP

1-octadecene C18H36[3, 4, 64]

Compound Data

Melting point	**17.17 °C**	**290.32 K**			
CSID	7925	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	252.4784	**H bond donors**	0	**ACD/LogP**	9.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	15	**Predicted density**	0.79 g/cm^3
SMILES	C=C\CCCCCCCCCCCCCCCC				
STD InChIKey	CCCMONHAUSKTEQ-UHFFFAOYAE				

Melting Points

mp °C	source
16.00	Alfa Aesar
18.00	American Petroleum Institute. Research Project 44; Selected ...
17.50	PHYSPROP

1-octadecyne C18H34[4, 64]

Compound Data

Melting point	**24.75 °C**	**297.90 K**			
CSID	62633	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	250.4626	**H bond donors**	0	**ACD/LogP**	8.97
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	0.81 g/cm^3
SMILES	C#CCCCCCCCCCCCCCCCC				
STD InChIKey	IYDNQWWOZQLMRH-UHFFFAOYAJ				

Melting Points

mp °C	source
27.00	American Petroleum Institute. Research Project 44; Selected ...
22.50	PHYSPROP

1-octanethiol C8H18S[3, 4, 64]

Compound Data

Melting point	**-49.07 °C**	**224.08 K**			
CSID	7852	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	146.2935	**H bond donors**	0	**ACD/LogP**	4.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.84 g/cm^3
SMILES	CCCCCCCCS				
STD InChIKey	KZCOBXFFBQJQHH-UHFFFAOYAI				

Melting Points

mp °C	source
-49.00	Alfa Aesar
-49.00	American Petroleum Institute. Research Project 44; Selected ...
-49.20	PHYSPROP

1-octanol C8H18O[3, 4, 64]

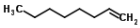
Compound Data

Melting point	**-15.50 °C**	**257.65 K**			
CSID	932	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	130.2279	**H bond donors**	1	**ACD/LogP**	2.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.82 g/cm^3
SMILES	CCCCCCCCO				
STD InChIKey	KBPLFHHGFOOTCA-UHFFFAOYAH				

Melting Points

mp °C	source
-16.00	Alfa Aesar
-15.00	American Petroleum Institute. Research Project 44; Selected ...
-15.50	PHYSPROP

1-octene C8H16[3, 4, 59, 64, 64]



Compound Data

Melting point	**-101.96 °C**	**171.19 K**			
CSID	7833	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.72 g/cm^3
SMILES	C=C\CCCCCC				
STD InChIKey	KWKAKUADMBZCLK-UHFFFAOYAN				

Melting Points

mp °C	source
-102.00	Alfa Aesar
-102.00	American Petroleum Institute. Research Project 44; Selected ...
-102.15	NIST Web Book
-101.70	PHYSPROP
	Values not used in calculating the average melting point
-109.00	PHYSPROP[1]

1. Value clearly out of range EC

1-octylamine C8H19N[3, 31, 35, 64]

Compound Data

Melting point	**-0.25 °C**	**272.90 K**			
CSID	7851	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.2432	**H bond donors**	2	**ACD/LogP**	3.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.79 g/cm^3
SMILES	NCCCCCCCC				
STD InChIKey	IOQPZZOEVPZRBK-UHFFFAOYAR				

Melting Points

mp °C	source
-1.00	Alfa Aesar
0.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
0.00	EPISuite-ChemSpider
0.00	PHYSPROP

1-pentadecanol C15H32O[2, 3, 64]

Compound Data

Melting point	**45.83 °C**	**318.98 K**			
CSID	11891	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	228.414	**H bond donors**	1	**ACD/LogP**	6.72
Phase 25 °C	solid	**Rotatable bonds**	14	**Predicted density**	0.83 g/cm^3
SMILES	OCCCCCCCCCCCCCCC				
STD InChIKey	REIUXOLGHVXAEO-UHFFFAOYAZ				

Melting Points

mp °C	source
46.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
46.00	Alfa Aesar
45.50	PHYSPROP

1-pentadecene C15H30[3, 4, 64]

Compound Data

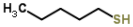
Melting point	**-3.60 °C**	**269.55 K**			
CSID	24142	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	210.3987	**H bond donors**	0	**ACD/LogP**	8.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	12	**Predicted density**	0.78 g/cm^3
SMILES	C=C\CCCCCCCCCCCCC				
STD InChIKey	PJLHTVIBELQURV-UHFFFAOYAF				

Melting Points

mp °C	source
-4.00	Alfa Aesar
-4.00	American Petroleum Institute. Research Project 44; Selected ...
-2.80	PHYSPROP

1-pentanethiol C5H12S[3, 4, 64]

Compound Data



Melting point	**-75.90 °C**	**197.25 K**			
CSID	7776	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	104.2138	**H bond donors**	0	**ACD/LogP**	2.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.83 g/cm^3
SMILES	SCCCCC				
STD InChIKey	ZRKMQKLGEQPLNS-UHFFFAOYAZ				

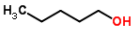
Melting Points

mp °C	source
-76.00	Alfa Aesar
-76.00	American Petroleum Institute. Research Project 44; Selected ...
-75.70	PHYSPROP

1-pentanol C5H12O[3, 4, 61, 64]

Compound Data

Melting point	**-78.47 °C**	**194.67 K**			
CSID	6040	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	1	**ACD/LogP**	1.41



Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.81 g/cm^3
SMILES	OCCCCC				
STD InChIKey	AMQJEAYHLZJPGS-UHFFFAOYAF				

Melting Points

mp °C	source
-79.00	Alfa Aesar
-78.00	American Petroleum Institute. Research Project 44; Selected ...
-78.00	Oxford University MSDS
-78.90	PHYSPROP

1-pentene C5H10[4, 28, 61, 64]

Compound Data

Melting point	**-164.33 °C**	**108.82 K**			
CSID	7713	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.85
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.66 g/cm^3
SMILES	CCCC=C				
STD InChIKey	YWAKXRMUMFPDSH-UHFFFAOYAJ				

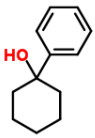
Melting Points

mp °C	source
-165.00	American Petroleum Institute. Research Project 44; Selected ...
-162.12	CRC Handbook of Chemistry and Physics
-165.00	Oxford University MSDS
-165.20	PHYSPROP
	Values not used in calculating the average melting point
-138.00	Alfa Aesar[1]

1. clearly out of range JCB

1-phenylcyclohexanol C12H16O[3, 64]

Compound Data



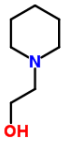
Melting point	**61.75 °C**	**334.90 K**			
CSID	14582	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	176.2548	**H bond donors**	1	**ACD/LogP**	2.94
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	OC2(c1ccccc1)CCCCC2				
STD InChIKey	DTTDXHDYTWQDCS-UHFFFAOYAO				

Melting Points

mp °C	source
60.00	Alfa Aesar
63.50	PHYSPROP

1-piperidineethanol C7H15NO[3, 64]

Compound Data



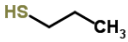
Melting point	**16.95 °C**	**290.10 K**			
CSID	17221	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	129.2001	**H bond donors**	1	**ACD/LogP**	1.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.97 g/cm^3
SMILES	OCCN1CCCCC1				
STD InChIKey	KZTWONRVIPPDKH-UHFFFAOYAQ				

Melting Points

mp °C	source
16.00	Alfa Aesar

17.90	PHYSPROP

1-propanethiol C3H8S[3, 4, 64]



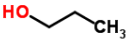
Compound Data

Melting point	**-113.10 °C**	**160.05 K**			
CSID	7560	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	76.1606	**H bond donors**	0	**ACD/LogP**	1.78
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.83 g/cm^3
SMILES	SCCC				
STD InChIKey	SUVIGLJNEAMWEG-UHFFFAOYAT				

Melting Points

mp °C	source
-113.00	Alfa Aesar
-113.00	American Petroleum Institute. Research Project 44; Selected ...
-113.30	PHYSPROP

1-propanol C3H8O[3, 4, 61, 64]



Compound Data

Melting point	**-126.53 °C**	**146.62 K**			
CSID	1004	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	60.095	**H bond donors**	1	**ACD/LogP**	0.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.80 g/cm^3
SMILES	CCCO				
STD InChIKey	BDERNNFJNOPAEC-UHFFFAOYAO				

Melting Points

mp °C	source
-127.00	Alfa Aesar
-126.00	American Petroleum Institute. Research Project 44; Selected ...
-127.00	Oxford University MSDS
-126.10	PHYSPROP

1-tetradecanol C14H30O[2, 3, 64]

Compound Data

Melting point	**39.50 °C**	**312.65 K**			
CSID	7917	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	214.3874	**H bond donors**	1	**ACD/LogP**	6.19
Phase 25 °C	solid	**Rotatable bonds**	13	**Predicted density**	0.83 g/cm^3
SMILES	OCCCCCCCCCCCCCC				
STD InChIKey	HLZKNKRTKFSKGZ-UHFFFAOYAP				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
39.00	Alfa Aesar
39.50	PHYSPROP

1-tetradecene C14H28[3, 4, 61, 64]

Compound Data

Melting point	**-12.50 °C**	**260.65 K**			
CSID	13622	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	196.3721	**H bond donors**	0	**ACD/LogP**	7.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.77 g/cm^3
SMILES	C=C\CCCCCCCCCCCC				
STD InChIKey	HFDVRLIODXPAHB-UHFFFAOYAK				

Melting Points

mp °C	source
-12.00	Alfa Aesar
-13.00	American Petroleum Institute. Research Project 44; Selected ...
-13.00	Oxford University MSDS
-12.00	PHYSPROP

1-tridecanol C13H28O[2, 64]

Compound Data

Melting point	**33.25 °C**	**306.40 K**			
CSID	7915	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	200.3608	**H bond donors**	1	**ACD/LogP**	5.66
Phase 25 °C	solid	**Rotatable bonds**	12	**Predicted density**	0.83 g/cm^3
SMILES	OCCCCCCCCCCCCC				
STD InChIKey	XFRVVPUIAFSTFO-UHFFFAOYAK				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.50	PHYSPROP

1,1-dichloroethane C2H4Cl2[31, 64]

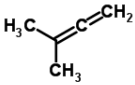
Compound Data

Melting point	**-96.95 °C**	**176.20 K**			
CSID	6125	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.9592	**H bond donors**	0	**ACD/LogP**	1.53
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.17 g/cm^3
SMILES	ClC(Cl)C				
STD InChIKey	SCYULBFZEHDVBN-UHFFFAOYAY				

Melting Points

mp °C	source
-97.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-96.90	PHYSPROP

1,1-dimethylallene C5H8[3, 64]



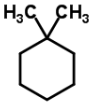
Compound Data

Melting point	**-113.80 °C**	**159.35 K**			
CSID	11222	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	68.117	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.65 g/cm^3
SMILES	C(=C)=C(\C)C				
STD InChIKey	PAKGDPSCXSUALC-UHFFFAOYAM				

Melting Points

mp °C	source
-114.00	Alfa Aesar
-113.60	PHYSPROP

1,1-dimethylcyclohexane C8H16[4, 64]



Compound Data

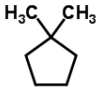
Melting point	**-33.15 °C**	**240.00 K**			
CSID	11062	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3
SMILES	CC1(C)CCCCC1				
STD InChIKey	QEGNUYASOUJEHD-UHFFFAOYAZ				

Melting Points

mp °C	source
-33.00	American Petroleum Institute. Research Project 44; Selected ...
-33.30	PHYSPROP

1,1-dimethylcyclopentane C7H14[4, 64]

Compound Data



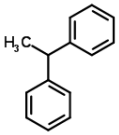
Melting point	**-69.90 °C**	**203.25 K**			
CSID	14679	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.85
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3
SMILES	CC1(C)CCCC1				
STD InChIKey	QWHNJUXXYKPLQM-UHFFFAOYAY				

Melting Points

mp °C	source
-70.00	American Petroleum Institute. Research Project 44; Selected ...
-69.80	PHYSPROP

1,1-diphenylethane C14H14[4, 64, 70]

Compound Data



Melting point	**-17.95 °C**	**255.20 K**			
CSID	11424	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.55
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.98 g/cm^3
SMILES	c1(ccccc1)C(c2ccccc2)C				
STD InChIKey	BSZXAFXFTLXUFV-UHFFFAOYAI				

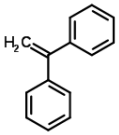
Melting Points

mp °C	source
-18.00	American Petroleum Institute. Research Project 44; Selected ...
-17.90	PHYSPROP
	Values not used in calculating the average melting point
25.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)[1]

1. value out of range of many other sources - EC

1,1-diphenylethylene C14H12[3, 4, 64]

Compound Data



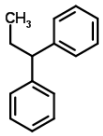
Melting point	**7.40 °C**	**280.55 K**			
CSID	10287	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	180.2451	**H bond donors**	0	**ACD/LogP**	3.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	C=C(c1ccccc1)c2ccccc2				
STD InChIKey	ZMYIIHDQURVDRB-UHFFFAOYAF				

Melting Points

mp °C	source
6.00	Alfa Aesar
8.00	American Petroleum Institute. Research Project 44; Selected ...
8.20	PHYSPROP

1,1-diphenylpropane C15H16[4, 64]

Compound Data



Melting point	**13.65 °C**	**286.80 K**			
CSID	66369	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	196.2875	**H bond donors**	0	**ACD/LogP**	5.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.97 g/cm^3
SMILES	c1ccccc1C(c2ccccc2)CC				

STD InChIKey	BUZMJVBOGDBMGI-UHFFFAOYAC

Melting Points

mp °C	source
14.00	American Petroleum Institute. Research Project 44; Selected ...
13.30	PHYSPROP

1,1,1-trichloroethane C2H3Cl3[31, 61, 64]

Compound Data

Melting point	**-31.14 °C**	**242.01 K**			
CSID	6042	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	133.4042	**H bond donors**	0	**ACD/LogP**	2.10
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	ClC(Cl)(Cl)C				
STD InChIKey	UOCLXMDMGBRAIB-UHFFFAOYAP				

Melting Points

mp °C	source
-30.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-33.00	Oxford University MSDS
-30.41	PHYSPROP

1,1,1-trifluoroethane C2H3F3[61, 64]

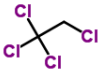
Compound Data

Melting point	**-111.15 °C**	**162.00 K**			
CSID	9484	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.0404	**H bond donors**	0	**ACD/LogP**	0.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	FC(F)(F)C				
STD InChIKey	UJPMYEOUBPIPHQ-UHFFFAOYAD				

Melting Points

mp °C	source
-111.00	Oxford University MSDS
-111.30	PHYSPROP

1,1,1,2-tetrachloroethane C2H2Cl4[31, 61, 64]



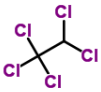
Compound Data

Melting point	**-70.07 °C**	**203.08 K**			
CSID	11911	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	167.8493	**H bond donors**	0	**ACD/LogP**	2.48
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.57 g/cm^3
SMILES	ClCC(Cl)(Cl)Cl				
STD InChIKey	QVLAWKAXOMEXPM-UHFFFAOYAE				

Melting Points

mp °C	source
-70.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-70.00	Oxford University MSDS
-70.20	PHYSPROP

1,1,1,2,2-pentachloroethane C2HCl5[3, 61, 64]



Compound Data

Melting point	**-28.93 °C**	**244.22 K**			
CSID	6179	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	202.2943	**H bond donors**	0	**ACD/LogP**	3.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.70 g/cm^3
SMILES	ClC(Cl)C(Cl)(Cl)Cl				

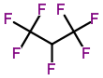
STD InChIKey	BNIXVQGCZULYKV-UHFFFAOYAS

Melting Points

mp °C	source
-29.00	Alfa Aesar
-29.00	Oxford University MSDS
-28.78	PHYSPROP

1,1,1,2,3,3,3-heptafluoropropane C3HF7[61, 64]

Compound Data



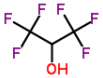
Melting point	**-129.05 °C**	**144.10 K**			
CSID	61257	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	170.0289	**H bond donors**	0	**ACD/LogP**	1.61
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.46 g/cm^3
SMILES	FC(F)(F)C(F)C(F)(F)F				
STD InChIKey	YFMFNYKEUDLDTL-UHFFFAOYAL				

Melting Points

mp °C	source
-131.00	Oxford University MSDS
-127.10	PHYSPROP

1,1,1,3,3,3-hexafluoropropan-2-ol C3H2F6O[3, 61, 64]

Compound Data



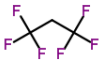
Melting point	**-3.33 °C**	**269.82 K**			
CSID	12941	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	168.0378	**H bond donors**	1	**ACD/LogP**	1.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	FC(F)(F)C(O)C(F)(F)F				
STD InChIKey	BYEAHWXPCBROCE-UHFFFAOYAH				

Melting Points

mp °C	source
-3.00	Alfa Aesar
-3.00	Oxford University MSDS
-4.00	PHYSPROP

1,1,1,3,3,3-hexafluoropropane C3H2F6[61, 64]

Compound Data



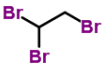
Melting point	**-96.10 °C**	**177.05 K**			
CSID	12199	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	152.0384	**H bond donors**	0	**ACD/LogP**	1.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.37 g/cm^3
SMILES	FC(F)(F)CC(F)(F)F				
STD InChIKey	NSGXIBWMJZWTPY-UHFFFAOYAC				

Melting Points

mp °C	source
-98.00	Oxford University MSDS
-94.20	PHYSPROP

1,1,2-tribromoethane C2H3Br3[31, 64]

Compound Data



Melting point	**-29.15 °C**	**244.00 K**			
CSID	59607	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	266.7572	**H bond donors**	0	**ACD/LogP**	2.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	2.63 g/cm^3
SMILES	BrC(Br)CBr				

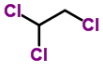
STD InChIKey	QUMDOMSJJIFTCA-UHFFFAOYAQ

Melting Points

mp °C	source
-29.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-29.30	PHYSPROP

1,1,2-trichloroethane C2H3Cl3[31, 61, 64]

Compound Data



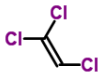
Melting point	**-36.20 °C**	**236.95 K**			
CSID	6326	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	133.4042	**H bond donors**	0	**ACD/LogP**	1.92
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	C(C(Cl)Cl)Cl				
STD InChIKey	UBOXGVDOUJQMTN-UHFFFAOYAA				

Melting Points

mp °C	source
-37.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-35.00	Oxford University MSDS
-36.60	PHYSPROP

1,1,2-trichloroethene C2HCl3[3, 61, 64]

Compound Data



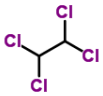
Melting point	**-84.90 °C**	**188.25 K**			
CSID	13837280	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	131.3883	**H bond donors**	0	**ACD/LogP**	2.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.47 g/cm^3
SMILES	Cl\C=C(/Cl)Cl				
STD InChIKey	XSTXAVWGXDQKEL-UHFFFAOYAI				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-85.00	Oxford University MSDS
-84.70	PHYSPROP

1,1,2,2-tetrachloroethane C2H2Cl4[3, 31, 61, 64]

Compound Data



Melting point	**-43.45 °C**	**229.70 K**			
CSID	6342	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	167.8493	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.56 g/cm^3
SMILES	ClC(Cl)C(Cl)Cl				
STD InChIKey	QPFMBZIOSGYJDE-UHFFFAOYAH				

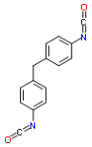
Melting Points

mp °C	source
-43.00	Alfa Aesar
-44.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-43.00	Oxford University MSDS
-43.80	PHYSPROP

1,1'-methylenebis(4-isocyanatobenzene) C15H10N2O2[61, 64]

Compound Data

Melting point	**37.60 °C**	**310.75 K**			
CSID	7289	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	250.2521	**H bond donors**	0	**ACD/LogP**	4.93



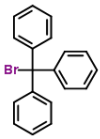
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm
SMILES	O=C=N\c1ccc(cc1)Cc2ccc(\N=C=O)cc2				
STD InChIKey	UPMLOUAZCHDJJD-UHFFFAOYAD				

Melting Points

mp °C	source
37.20	Oxford University MSDS
38.00	PHYSPROP

1,1',1''-(bromomethanetriyl)tribenzene C19H15Br[3, 61, 64]

Compound Data



Melting point	**153.33 °C**	**426.48 K**			
CSID	11200	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	323.2264	**H bond donors**	0	**ACD/LogP**	6.51
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.31 g/cm^3
SMILES	BrC(c1ccccc1)(c2ccccc2)c3ccccc3				
STD InChIKey	NZHXEWZGTQSYJM-UHFFFAOYAC				

Melting Points

mp °C	source
154.00	Alfa Aesar
153.00	Oxford University MSDS
153.00	PHYSPROP

1,10-decanediol C10H22O2[3, 61, 64]

Compound Data

Melting point	**73.00 °C**	**346.15 K**			
CSID	34095	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	174.2805	**H bond donors**	2	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	11	**Predicted density**	0.92 g/cm^3
SMILES	OCCCCCCCCCCCO				
STD InChIKey	FOTKYAAJKYLFFN-UHFFFAOYAW				

Melting Points

mp °C	source
73.00	Alfa Aesar
72.00	Oxford University MSDS
74.00	PHYSPROP

1,12-dibromododecane C12H24Br2[3, 64]

Compound Data

Melting point	**40.50 °C**	**313.65 K**			
CSID	17720	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	328.127	**H bond donors**	0	**ACD/LogP**	6.85
Phase 25 °C	solid	**Rotatable bonds**	11	**Predicted density**	1.30 g/cm^3
SMILES	BrCCCCCCCCCCCCBr				
STD InChIKey	ZJJATABWMGVVRZ-UHFFFAOYAU				

Melting Points

mp °C	source
40.00	Alfa Aesar
41.00	PHYSPROP

1,12-dodecanediol C12H26O2[3, 64]

Compound Data

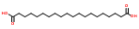
Melting point	**82.15 °C**	**355.30 K**			
CSID	72056	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	202.3336	**H bond donors**	2	**ACD/LogP**	3.12
Phase 25 °C	solid	**Rotatable bonds**	13	**Predicted density**	0.91 g/cm^3
SMILES	OCCCCCCCCCCCCCO				
STD InChIKey	GHLKSLMMWAKNBM-UHFFFAOYAY				

Melting Points

mp °C	source
83.00	Alfa Aesar
81.30	PHYSPROP

1,18-octadecanedicarboxylic acid C20H38O4[3, 64]

Compound Data



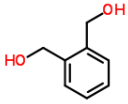
Melting point	**126.25 °C**	**399.40 K**			
CSID	68030	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	342.5133	**H bond donors**	2	**ACD/LogP**	7.17
Phase 25 °C	solid	**Rotatable bonds**	19	**Predicted density**	0.98 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCCCCCCC(=O)O				
STD InChIKey	JJOJFIHJIRWASH-UHFFFAOYAR				

Melting Points

mp °C	source
127.00	Alfa Aesar
125.50	PHYSPROP

1,2-benzenedimethanol C8H10O2[2, 3]

Compound Data



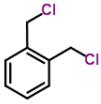
Melting point	**63.00 °C**	**336.15 K**			
CSID	62368	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	2	**ACD/LogP**	0.02
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	OCc1ccccc1CO				
STD InChIKey	XMUZQOKACOLCSS-UHFFFAOYAW				

Melting Points

mp °C	source
64.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
62.00	Alfa Aesar

1,2-bis-(chloromethyl)xylene C8H8Cl2[2, 3, 64]

Compound Data



Melting point	**55.33 °C**	**328.48 K**			
CSID	21111896	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	175.0551	**H bond donors**	0	**ACD/LogP**	2.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	ClCc1ccccc1CCl				
STD InChIKey	FMGGHNGKHRCJLL-UHFFFAOYAV				

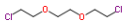
Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
55.00	PHYSPROP

1,2-bis(2-chloroethoxy)ethane C6H12Cl2O2[3, 64]

Compound Data

Melting point	**-31.75 °C**	**241.40 K**



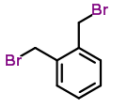
CSID	7879	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	187.0643	**H bond donors**	0	**ACD/LogP**	0.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.15 g/cm^3
SMILES	ClCCOCCOCCCl				
STD InChIKey	AGYUOJIYYGGHKV-UHFFFAOYAM				

Melting Points

mp °C	source
-32.00	Alfa Aesar
-31.50	PHYSPROP

1,2-bis(bromomethyl)benzene C8H8Br2[3, 64]

Compound Data



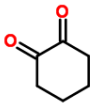
Melting point	**94.50 °C**	**367.65 K**			
CSID	60032	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	263.9571	**H bond donors**	0	**ACD/LogP**	3.70
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.78 g/cm^3
SMILES	BrCc1ccccc1CBr				
STD InChIKey	KGKAYWMGPDWLQZ-UHFFFAOYAZ				

Melting Points

mp °C	source
94.00	Alfa Aesar
95.00	PHYSPROP

1,2-cyclohexanedione C6H8O2[3, 64]

Compound Data



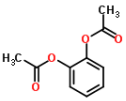
Melting point	**38.50 °C**	**311.65 K**			
CSID	12465	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	112.1265	**H bond donors**	0	**ACD/LogP**	0.11
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	O=C1C(=O)CCCC1				
STD InChIKey	OILAIQUEIWYQPH-UHFFFAOYAM				

Melting Points

mp °C	source
37.00	Alfa Aesar
40.00	PHYSPROP

1,2-diacetoxybenzene C10H10O4[7, 64]

Compound Data



Melting point	**64.25 °C**	**337.40 K**			
CSID	11969	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	0.54
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(Oc1ccccc1OC(=O)C)C				
STD InChIKey	FBSAITBEAPNWJG-UHFFFAOYAE				

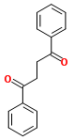
Melting Points

mp °C	source
64.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
64.50	PHYSPROP

1,2-dibenzoylethane C16H14O2[3, 48]

Compound Data

Melting point	**145.00 °C**	**418.15 K**			
CSID	120096	**H bond acceptors**	2	**Rule of 5 violations**	0



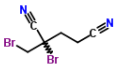
Molecular weight	238.2812	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.12 g/cm^3
SMILES	O=C(c1ccccc1)CCC(=O)c2ccccc2				
STD InChIKey	OSWWFLDIIGGSJV-UHFFFAOYAU				

Melting Points

mp °C	source
146.00	Alfa Aesar
144.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

1,2-dibromo-2,4-dicyanobutane C6H6Br2N2[3, 64]

Compound Data



Melting point	**51.00 °C**	**324.15 K**			
CSID	55806	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	265.9332	**H bond donors**	0	**ACD/LogP**	1.71
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.89 g/cm^3
SMILES	N#CCCC(Br)(C#N)CBr				
STD InChIKey	DHVLDKHFGIVEIP-UHFFFAOYAK				

Melting Points

mp °C	source
50.00	Alfa Aesar
52.00	PHYSPROP

1,2-dibromobenzene C6H4Br2[3, 31, 64]

Compound Data

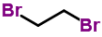
Melting point	**6.37 °C**	**279.52 K**			
CSID	13875212	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	235.904	**H bond donors**	0	**ACD/LogP**	3.63
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.94 g/cm^3
SMILES	Brc1ccccc1Br				
STD InChIKey	WQONPSCCEXUXTQ-UHFFFAOYAQ				

Melting Points

mp °C	source
5.00	Alfa Aesar
7.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
7.10	PHYSPROP

1,2-dibromoethane C2H4Br2[3, 31, 64]

Compound Data



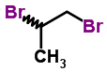
Melting point	**9.97 °C**	**283.12 K**			
CSID	7551	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	187.8612	**H bond donors**	0	**ACD/LogP**	2.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	2.14 g/cm^3
SMILES	BrCCBr				
STD InChIKey	PAAZPARNPHGIKF-UHFFFAOYAZ				

Melting Points

mp °C	source
10.00	Alfa Aesar
10.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
9.90	PHYSPROP

1,2-dibromopropane C3H6Br2[3, 31, 64]

Compound Data



Melting point	**-55.16 °C**	**217.99 K**			
CSID	6305	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	201.8877	**H bond donors**	0	**ACD/LogP**	2.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.93 g/cm^3
SMILES	BrC(C)CBr				
STD InChIKey	XFNJYAKDBJUJAJ-UHFFFAOYAK				

Melting Points

mp °C	source
-55.00	Alfa Aesar
-55.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-55.49	PHYSPROP

1,2-dichloro-4-nitrobenzene C6H3Cl2NO2[2, 3, 61, 64, 70]

Compound Data

Melting point	**41.00 °C**	**314.15 K**			
CSID	21106095	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.9995	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3
SMILES	Clc1ccc(cc1Cl)[N+]([O-])=O				
STD InChIKey	NTBYINQTYWZXLH-UHFFFAOYAQ				

Melting Points

mp °C	source
41.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
41.00	Alfa Aesar
39.00	Oxford University MSDS
43.00	PHYSPROP
41.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2-dichlorobenzene C6H4Cl2[3, 31, 64]

Compound Data

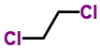
Melting point	**-17.23 °C**	**255.92 K**			
CSID	13837988	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	147.002	**H bond donors**	0	**ACD/LogP**	3.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.30 g/cm^3
SMILES	c1ccc(c(c1)Cl)Cl				
STD InChIKey	RFFLAFLAYFXFSW-UHFFFAOYAE				

Melting Points

mp °C	source
-18.00	Alfa Aesar
-17.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-16.70	PHYSPROP

1,2-dichloroethane C2H4Cl2[3, 31, 64]

Compound Data



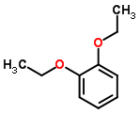
Melting point	**-35.50 °C**	**237.65 K**			
CSID	13837650	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.9592	**H bond donors**	0	**ACD/LogP**	1.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	ClCCCl				
STD InChIKey	WSLDOOZREJYCGB-UHFFFAOYAL				

Melting Points

mp °C	source
-35.00	Alfa Aesar
-36.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-35.50	PHYSPROP

1,2-diethoxybenzene $C_{10}H_{14}O_2$[3, 7, 64]

Compound Data



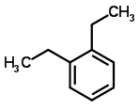
Melting point	**43.67 °C**	**316.82 K**			
CSID	67466	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	166.217	**H bond donors**	0	**ACD/LogP**	3.02
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.97 g/cm^3
SMILES	O(c1ccccc1OCC)CC				
STD InChIKey	QZYDOKBVZJLQCK-UHFFFAOYAU				

Melting Points

mp °C	source
44.00	Alfa Aesar
43.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
44.00	PHYSPROP

1,2-diethylbenzene $C_{10}H_{14}$[3, 4, 64]

Compound Data



Melting point	**-31.07 °C**	**242.08 K**			
CSID	8335	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.86 g/cm^3
SMILES	c1cccc(c1CC)CC				
STD InChIKey	KVNYFPKFSJIPBJ-UHFFFAOYAM				

Melting Points

mp °C	source
-31.00	Alfa Aesar
-31.00	American Petroleum Institute. Research Project 44; Selected ...
-31.20	PHYSPROP

1,2-diiodoethane $C_2H_4I_2$[3, 31, 61, 64]

Compound Data

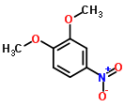
Melting point	**81.50 °C**	**354.65 K**			
CSID	11723	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	281.8621	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.84 g/cm^3
SMILES	ICCI				
STD InChIKey	GBBZLMLLFVFKJM-UHFFFAOYAR				

Melting Points

mp °C	source
82.00	Alfa Aesar
81.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
80.00	Oxford University MSDS
83.00	PHYSPROP

1,2-dimethoxy-4-nitrobenzene $C_8H_9NO_4$[2, 3, 64]

Compound Data



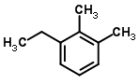
Melting point	**97.33 °C**	**370.48 K**			
CSID	62928	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	183.1614	**H bond donors**	0	**ACD/LogP**	2.16
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	[O-][N+](=O)c1cc(OC)c(OC)cc1				
STD InChIKey	YFWBUVZWCBFSQN-UHFFFAOYAI				

Melting Points

mp °C	source
97.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

97.00	Alfa Aesar
98.00	PHYSPROP

1,2-dimethyl-3-ethylbenzene C10H14[4, 64]



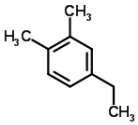
Compound Data

Melting point	**-49.75 °C**	**223.40 K**			
CSID	13032	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1(cccc(c1C)CC)C				
STD InChIKey	QUBBAXISAHIDNM-UHFFFAOYAP				

Melting Points

mp °C	source
-50.00	American Petroleum Institute. Research Project 44; Selected ...
-49.50	PHYSPROP

1,2-dimethyl-4-ethylbenzene C10H14[4, 64]



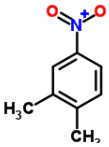
Compound Data

Melting point	**-66.95 °C**	**206.20 K**			
CSID	13040	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1c(ccc(c1C)C)CC				
STD InChIKey	SBUYFICWQNHBCM-UHFFFAOYAE				

Melting Points

mp °C	source
-67.00	American Petroleum Institute. Research Project 44; Selected ...
-66.90	PHYSPROP

1,2-dimethyl-4-nitrobenzene C8H9NO2[2, 3, 61, 64]



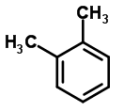
Compound Data

Melting point	**30.25 °C**	**303.40 K**			
CSID	7162	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	[O-][N+](=O)c1cc(c(cc1)C)C				
STD InChIKey	HFZKOYWDLDYELC-UHFFFAOYAU				

Melting Points

mp °C	source
31.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
29.00	Alfa Aesar
30.50	Oxford University MSDS
30.50	PHYSPROP

1,2-dimethylbenzene C8H10[3, 4, 64]



Compound Data

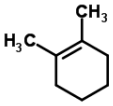
Melting point	**-25.07 °C**	**248.08 K**			
CSID	6967	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.165	**H bond donors**	0	**ACD/LogP**	3.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	Cc1ccccc1C				
STD InChIKey	CTQNGGLPUBDAKN-UHFFFAOYAE				

Melting Points

mp °C	source

-25.00	Alfa Aesar
-25.00	American Petroleum Institute. Research Project 44; Selected ...
-25.20	PHYSPROP

1,2-dimethylcyclohexene C8H14[4, 64]



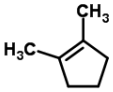
Compound Data

Melting point	**-84.05 °C**	**189.10 K**			
CSID	14729	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	4.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.81 g/cm^3
SMILES	C1(=C(\C)CCCC1)\C				
STD InChIKey	TXNWMICHNKMOBR-UHFFFAOYAI				

Melting Points

mp °C	source
-84.00	American Petroleum Institute. Research Project 44; Selected ...
-84.10	PHYSPROP

1,2-dimethylcyclopentene C7H12[4, 64]



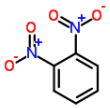
Compound Data

Melting point	**-90.20 °C**	**182.95 K**			
CSID	63026	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	3.51
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.81 g/cm^3
SMILES	C1(=C(\C)CCC1)\C				
STD InChIKey	SZZWLAZADBEDQP-UHFFFAOYAX				

Melting Points

mp °C	source
-90.00	American Petroleum Institute. Research Project 44; Selected ...
-90.40	PHYSPROP

1,2-dinitrobenzene C6H4N2O4[2, 64]



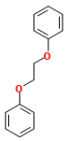
Compound Data

Melting point	**118.25 °C**	**391.40 K**			
CSID	10257	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	168.107	**H bond donors**	0	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.49 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1[N+]([O-])=O				
STD InChIKey	IZUKQUVSCNEFMJ-UHFFFAOYAA				

Melting Points

mp °C	source
118.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
118.50	PHYSPROP

1,2-diphenoxyethane C14H14O2[2, 3, 64]



Compound Data

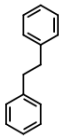
Melting point	**96.00 °C**	**369.15 K**			
CSID	7427	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	214.2598	**H bond donors**	0	**ACD/LogP**	3.81
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.08 g/cm^3
SMILES	O(c1ccccc1)CCOc2ccccc2				
STD InChIKey	XCSGHNKDXGYELG-UHFFFAOYAH				

Melting Points

mp °C	source
95.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

95.00	Alfa Aesar
98.00	PHYSPROP

1,2-diphenylethane C14H14[3, 4, 48, 64, 70]



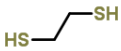
Compound Data

Melting point	**52.50 °C**	**325.65 K**			
CSID	7364	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.61
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.00 g/cm^3
SMILES	c1ccc(cc1)CCc2ccccc2				
STD InChIKey	QWUWMCYKGHVNAV-UHFFFAOYAL				

Melting Points

mp °C	source
52.00	Alfa Aesar
51.00	American Petroleum Institute. Research Project 44; Selected ...
55.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
52.50	PHYSPROP
52.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2-ethanedithiol C2H6S2[3, 61, 64]



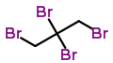
Compound Data

Melting point	**-41.07 °C**	**232.08 K**			
CSID	13865015	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	94.199	**H bond donors**	0	**ACD/LogP**	1.31
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3
SMILES	SCCS				
STD InChIKey	VYMPLPIFKRHAAC-UHFFFAOYAA				

Melting Points

mp °C	source
-41.00	Alfa Aesar
-41.00	Oxford University MSDS
-41.20	PHYSPROP

1,2,2,3-tetrabromopropane C3H4Br4[31, 64]



Compound Data

Melting point	**10.75 °C**	**283.90 K**			
CSID	37466	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	359.6799	**H bond donors**	0	**ACD/LogP**	4.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	2.75 g/cm^3
SMILES	BrC(Br)(CBr)CBr				
STD InChIKey	SNLFZAHVOKOBOP-UHFFFAOYAP				

Melting Points

mp °C	source
11.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
10.50	PHYSPROP

1,2,3-triazole C2H3N3[3, 61, 64, 72]

Compound Data

Melting point	**23.67 °C**	**296.82 K**			
CSID	60839	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	69.0653	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	c1cnn[nH]1				
STD InChIKey	QWENRTYMTSOGBR-UHFFFAOYAF				

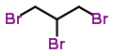
Melting Points

mp °C	source
24.00	Alfa Aesar
23.00	PHYSPROP
24.00	Sigma-Aldrich
	Values not used in calculating the average melting point
167.00	Oxford University MSDS[1]

1. clearly out of range JCB

1,2,3-tribromopropane C3H5Br3[3, 31, 64]

Compound Data



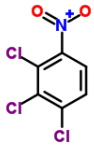
Melting point	**16.63 °C**	**289.78 K**			
CSID	7007	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	280.7838	**H bond donors**	0	**ACD/LogP**	3.31
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	2.38 g/cm^3
SMILES	BrC(CBr)CBr				
STD InChIKey	FHCLGDLYRUPKAM-UHFFFAOYAE				

Melting Points

mp °C	source
17.00	Alfa Aesar
16.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
16.90	PHYSPROP

1,2,3-trichloro-4-nitrobenzene C6H2Cl3NO2[3, 64, 70]

Compound Data



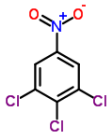
Melting point	**55.50 °C**	**328.65 K**			
CSID	26691	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.4446	**H bond donors**	0	**ACD/LogP**	3.44
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.65 g/cm^3
SMILES	Clc1ccc([N+](O-])=O)c(Cl)c1Cl				
STD InChIKey	BGKIECJVXXHLDP-UHFFFAOYAO				

Melting Points

mp °C	source
55.00	Alfa Aesar
55.50	PHYSPROP
56.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2,3-trichloro-5-nitrobenzene C6H2Cl3NO2[3, 64]

Compound Data



Melting point	**71.25 °C**	**344.40 K**			
CSID	79719	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.4446	**H bond donors**	0	**ACD/LogP**	3.74
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.65 g/cm^3
SMILES	Clc1cc([N+](O-])=O)cc(Cl)c1Cl				
STD InChIKey	HHLCSFGOTLUREE-UHFFFAOYAS				

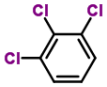
Melting Points

mp °C	source
70.00	Alfa Aesar
72.50	PHYSPROP

1,2,3-trichlorobenzene C6H3Cl3[2, 3, 44, 64, 70]

Compound Data

Melting point	**53.62 °C**	**326.77 K**			
CSID	13864445	**H bond acceptors**	0	**Rule of 5 violations**	0



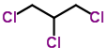
Molecular weight	181.447	**H bond donors**	0	**ACD/LogP**	3.77
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.45 g/cm^3
SMILES	Clc1cccc(Cl)c1Cl				
STD InChIKey	RELMFMZEBKVZJC-UHFFFAOYAX				

Melting Points

mp °C	source
55.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
52.60	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
53.50	PHYSPROP
53.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2,3-trichloropropane C3H5Cl3[3, 31, 64]

Compound Data



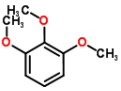
Melting point	**-14.57 °C**	**258.58 K**			
CSID	7013	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	147.4308	**H bond donors**	0	**ACD/LogP**	1.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	ClCC(Cl)CCl				
STD InChIKey	CFXQEHVMCRXUSD-UHFFFAOYAC				

Melting Points

mp °C	source
-14.00	Alfa Aesar
-15.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-14.70	PHYSPROP

1,2,3-trimethoxybenzene C9H12O3[2, 3, 64]

Compound Data



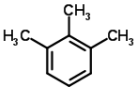
Melting point	**45.83 °C**	**318.98 K**			
CSID	21111804	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	168.1898	**H bond donors**	0	**ACD/LogP**	1.66
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.04 g/cm^3
SMILES	COc1c(cccc1OC)OC				
STD InChIKey	CRUILBNAQILVHZ-UHFFFAOYAP				

Melting Points

mp °C	source
45.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
44.00	Alfa Aesar
48.50	PHYSPROP

1,2,3-trimethylbenzene C9H12[2, 4, 61, 64]

Compound Data



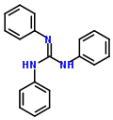
Melting point	**-25.10 °C**	**248.05 K**			
CSID	10236	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.1916	**H bond donors**	0	**ACD/LogP**	3.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1(cccc(c1C)C)C				
STD InChIKey	FYGHSUNMUKGBRK-UHFFFAOYAK				

Melting Points

mp °C	source
-25.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-25.00	American Petroleum Institute. Research Project 44; Selected ...
-25.00	Oxford University MSDS

-25.40	PHYSPROP

1,2,3-triphenylguanidine C19H17N3[3, 64]



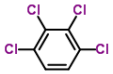
Compound Data

Melting point	**145.25 °C**	**418.40 K**			
CSID	7258	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	287.3584	**H bond donors**	2	**ACD/LogP**	4.94
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	N(=C(/Nc1ccccc1)Nc2ccccc2)\c3ccccc3				
STD InChIKey	FUPAJKKAHDLPAZ-UHFFFAOYAR				

Melting Points

mp °C	source
144.00	Alfa Aesar
146.50	PHYSPROP

1,2,3,4-tetrachlorobenzene C6H2Cl4[2, 64]



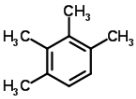
Compound Data

Melting point	**47.25 °C**	**320.40 K**			
CSID	21106540	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	215.8921	**H bond donors**	0	**ACD/LogP**	4.17
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.57 g/cm^3
SMILES	Clc1ccc(Cl)c(Cl)c1Cl				
STD InChIKey	GBDZXPJXOMHESU-UHFFFAOYAT				

Melting Points

mp °C	source
47.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
47.50	PHYSPROP

1,2,3,4-tetramethylbenzene C10H14[4, 64]



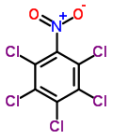
Compound Data

Melting point	**-6.10 °C**	**267.05 K**			
CSID	9844	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1(ccc(c(c1C)C)C)C				
STD InChIKey	UOHMMEJUHBCKEE-UHFFFAOYAP				

Melting Points

mp °C	source
-6.00	American Petroleum Institute. Research Project 44; Selected ...
-6.20	PHYSPROP

1,2,3,4,5-pentachloro-6-nitrobenzene C6Cl5NO2[61, 64]



Compound Data

Melting point	**142.75 °C**	**415.90 K**			
CSID	6464	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	295.3347	**H bond donors**	0	**ACD/LogP**	4.16
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.83 g/cm^3
SMILES	Clc1c(c(Cl)c(Cl)c(Cl)c1Cl)[N+](=[O-])=O				
STD InChIKey	LKPLKUMXSAEKID-UHFFFAOYAW				

Melting Points

mp °C	source
141.50	Oxford University MSDS
144.00	PHYSPROP

1,2,3,4,5-pentafluorobenzene C6HF5[61, 64]

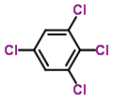
Compound Data

Melting point	**-47.65 °C**	**225.50 K**			
CSID	13866746	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	168.0642	**H bond donors**	0	**ACD/LogP**	2.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.52 g/cm^3
SMILES	Fc1cc(F)c(F)c(F)c1F				
STD InChIKey	WACNXHCZHTVBJM-UHFFFAOYAM				

Melting Points

mp °C	source
-48.00	Oxford University MSDS
-47.30	PHYSPROP

1,2,3,5-tetrachlorobenzene C6H2Cl4[2, 64, 70]



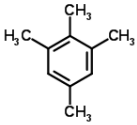
Compound Data

Melting point	**54.17 °C**	**327.32 K**			
CSID	21106571	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	215.8921	**H bond donors**	0	**ACD/LogP**	4.31
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.57 g/cm^3
SMILES	Clc1cc(Cl)c(Cl)c(Cl)c1				
STD InChIKey	QZYNWJQFTJXIRN-UHFFFAOYAM				

Melting Points

mp °C	source
53.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.50	PHYSPROP
55.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2,3,5-tetramethylbenzene C10H14[4, 64]



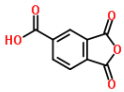
Compound Data

Melting point	**-23.85 °C**	**249.30 K**			
CSID	10245	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1(cc(cc(c1C)C)C)C				
STD InChIKey	BFIMMTCNYPIMRN-UHFFFAOYAG				

Melting Points

mp °C	source
-24.00	American Petroleum Institute. Research Project 44; Selected ...
-23.70	PHYSPROP

1,2,4-benzenetricarboxylic anhydride C9H4O5[3, 64]



Compound Data

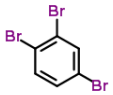
Melting point	**164.50 °C**	**437.65 K**			
CSID	10618	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	192.1251	**H bond donors**	1	**ACD/LogP**	1.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.67 g/cm^3
SMILES	O=C(O)c1ccc2C(=O)OC(=O)c2c1				
STD InChIKey	SRPWOOOHEPICQU-UHFFFAOYAL				

Melting Points

mp °C	source
167.00	Alfa Aesar
162.00	PHYSPROP

1,2,4-tribromobenzene C6H3Br3[2, 3, 64, 70]

Compound Data



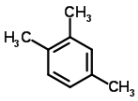
Melting point	**43.12 °C**	**316.27 K**			
CSID	11507	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	314.8	**H bond donors**	0	**ACD/LogP**	4.38
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.28 g/cm^3
SMILES	Brc1cc(Br)c(Br)cc1				
STD InChIKey	FWAJPSIPOULHHH-UHFFFAOYAX				

Melting Points

mp °C	source
43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
42.00	Alfa Aesar
44.50	PHYSPROP
43.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2,4-trimethylbenzene C9H12[3, 4, 61, 64]

Compound Data



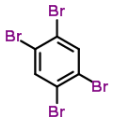
Melting point	**-43.90 °C**	**229.25 K**			
CSID	6977	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.1916	**H bond donors**	0	**ACD/LogP**	3.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1c(ccc(c1C)C)C				
STD InChIKey	GWHJZXXIDMPWGX-UHFFFAOYAF				

Melting Points

mp °C	source
-44.00	Alfa Aesar
-44.00	American Petroleum Institute. Research Project 44; Selected ...
-43.80	Oxford University MSDS
-43.80	PHYSPROP

1,2,4,5-tetrabromobenzene C6H2Br4[3, 64, 70]

Compound Data



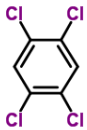
Melting point	**180.67 °C**	**453.82 K**			
CSID	11974	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	393.6961	**H bond donors**	0	**ACD/LogP**	5.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.55 g/cm^3
SMILES	Brc1c(Br)cc(Br)c(Br)c1				
STD InChIKey	QCKHVNQHBOGZER-UHFFFAOYAI				

Melting Points

mp °C	source
178.00	Alfa Aesar
182.00	PHYSPROP
182.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2,4,5-tetrachlorobenzene C6H2Cl4[2, 3, 61, 64, 70, 70]

Compound Data



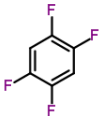
Melting point	**139.42 °C**	**412.57 K**			
CSID	21106163	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	215.8921	**H bond donors**	0	**ACD/LogP**	4.70
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.57 g/cm^3
SMILES	c1c(c(cc(c1Cl)Cl)Cl)Cl				
STD InChIKey	JHBKHLUZVFWLAG-UHFFFAOYAS				

Melting Points

mp °C	source
140.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
140.00	Alfa Aesar

139.00	Oxford University MSDS
139.50	PHYSPROP
139.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
139.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,2,4,5-tetrafluorobenzene C6H2F4[3, 64]



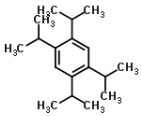
Compound Data

Melting point	**4.25 °C**	**277.40 K**			
CSID	21108549	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	150.0737	**H bond donors**	0	**ACD/LogP**	2.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.41 g/cm^3
SMILES	Fc1c(F)cc(F)c(F)c1				
STD InChIKey	SDXUIOOHCIQXRP-UHFFFAOYAJ				

Melting Points

mp °C	source
4.00	Alfa Aesar
4.50	PHYSPROP

1,2,4,5-tetraisopropylbenzene C18H30[7, 64]



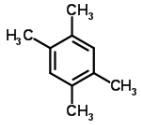
Compound Data

Melting point	**118.70 °C**	**391.85 K**			
CSID	62663	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	246.4308	**H bond donors**	0	**ACD/LogP**	7.57
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.85 g/cm^3
SMILES	c1c(c(cc(c1C(C)C)C(C)C)C(C)C)C(C)C				
STD InChIKey	ROXLYQQDLJJEBE-UHFFFAOYAD				

Melting Points

mp °C	source
119.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
118.40	PHYSPROP

1,2,4,5-tetramethylbenzene C10H14[2, 3, 64]



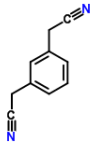
Compound Data

Melting point	**79.43 °C**	**352.58 K**			
CSID	6999	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.06
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1c(c(cc(c1C)C)C)C				
STD InChIKey	SQNZJJAZBFDUTD-UHFFFAOYAJ				

Melting Points

mp °C	source
80.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
79.00	Alfa Aesar
79.30	PHYSPROP

1,3-benzenediacetonitrile C10H8N2[2, 3, 64]



Compound Data

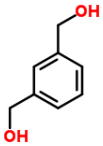
Melting point	**33.50 °C**	**306.65 K**			
CSID	62583	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.1839	**H bond donors**	0	**ACD/LogP**	0.68
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.10 g/cm^3
SMILES	N#CCc1cccc(c1)CC#N				
STD InChIKey	GRPFZJNUYXIVSL-UHFFFAOYAK				

Melting Points

mp °C	source
33.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
34.00	Alfa Aesar
33.50	PHYSPROP

1,3-benzenedimethanol C8H10O2[2, 3, 64]

Compound Data



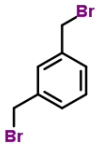
Melting point	**57.67 °C**	**330.82 K**			
CSID	62582	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	2	**ACD/LogP**	-0.15
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	OCc1cccc(c1)CO				
STD InChIKey	YWMLORGQOFONNT-UHFFFAOYAD				

Melting Points

mp °C	source
58.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
58.00	Alfa Aesar
57.00	PHYSPROP

1,3-benzenedimethanol C8H8Br2[3, 64]

Compound Data



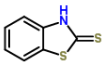
Melting point	**76.00 °C**	**349.15 K**			
CSID	62581	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	263.9571	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.78 g/cm^3
SMILES	BrCc1cccc(c1)CBr				
STD InChIKey	OXHOPZLBSSTTBU-UHFFFAOYAU				

Melting Points

mp °C	source
75.00	Alfa Aesar
77.00	PHYSPROP

1,3-benzothiazole-2-thiol C7H5NS2[3, 61, 64]

Compound Data



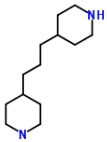
Melting point	**180.00 °C**	**453.15 K**			
CSID	608157	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	167.2513	**H bond donors**	1	**ACD/LogP**	2.38
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.46 g/cm^3
SMILES	S=C2Sc1ccccc1N2				
STD InChIKey	YXIWHUQXZSMYRE-UHFFFAOYAK				

Melting Points

mp °C	source
180.00	Alfa Aesar
179.00	Oxford University MSDS
181.00	PHYSPROP

1,3-bis(4-piperidinyl)propane C13H26N2[3, 64]

Compound Data



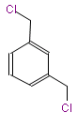
Melting point	**66.55 °C**	**339.70 K**			
CSID	77230	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	210.3589	**H bond donors**	2	**ACD/LogP**	2.62
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.89 g/cm^3
SMILES	N2CCC(CCCC1CCNCC1)CC2				
STD InChIKey	OXEZLYIDQPBCBB-UHFFFAOYAP				

Melting Points

mp °C	source
66.00	Alfa Aesar
67.10	PHYSPROP

1,3-bis(chlormethyl)benzene C8H8Cl2[2, 3, 64]

Compound Data



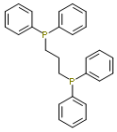
Melting point	**35.07 °C**	**308.22 K**			
CSID	21168838	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	175.0551	**H bond donors**	0	**ACD/LogP**	2.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	ClCc1cccc(CCl)c1				
STD InChIKey	GRJWOKACBGZOKT-UHFFFAOYAO				

Melting Points

mp °C	source
36.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
35.00	Alfa Aesar
34.20	PHYSPROP

1,3-bis(diphenylphosphino)propane C27H26P2[3, 48]

Compound Data



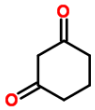
Melting point	**60.50 °C**	**333.65 K**			
CSID	73276	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	412.4429	**H bond donors**	0	**ACD/LogP**	6.98
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	0.00 g/cm^3
SMILES	c1ccc(cc1)P(CCCP(c2ccccc2)c3ccccc3)c4ccccc4				
STD InChIKey	LVEYOSJUKRVCCF-UHFFFAOYAP				

Melting Points

mp °C	source
61.00	Alfa Aesar
60.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

1,3-cyclohexanedione C6H8O2[3, 64]

Compound Data



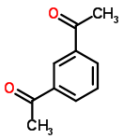
Melting point	**104.25 °C**	**377.40 K**			
CSID	10004	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	112.1265	**H bond donors**	0	**ACD/LogP**	-0.89
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	O=C1CCCC(=O)C1				
STD InChIKey	HJSLFCCWAKVHIW-UHFFFAOYAR				

Melting Points

mp °C	source
103.00	Alfa Aesar
105.50	PHYSPROP

1,3-diacetylbenzene C10H10O2[2, 3, 48, 64]

Compound Data

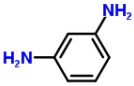


Melting point	**34.00 °C**	**307.15 K**			
CSID	21733	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	162.1852	**H bond donors**	0	**ACD/LogP**	1.43
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	O=C(c1cccc(C(=O)C)c1)C				
STD InChIKey	VCHOFVSNWYPAEF-UHFFFAOYAS				

Melting Points

mp °C	source
36.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
36.00	Alfa Aesar
32.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
32.00	PHYSPROP

1,3-diaminobenzene C6H8N2[2, 3, 64]



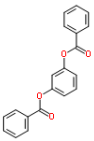
Compound Data

Melting point	**63.83 °C**	**336.98 K**			
CSID	13836283	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	4	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	Nc1cccc(N)c1				
STD InChIKey	WZCQRUWWHSTZEM-UHFFFAOYAM				

Melting Points

mp °C	source
65.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
63.00	Alfa Aesar
63.50	PHYSPROP

1,3-dibenzoyloxybenzene C20H14O4[3, 41, 64]



Compound Data

Melting point	**117.00 °C**	**390.15 K**			
CSID	60108	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	318.3228	**H bond donors**	0	**ACD/LogP**	4.96
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.24 g/cm^3
SMILES	O=C(Oc2cccc(OC(=O)c1ccccc1)c2)c3ccccc3				
STD InChIKey	SUQGLJRNDJRARS-UHFFFAOYAL				

Melting Points

mp °C	source
118.00	Alfa Aesar
116.00	GlobalChems
	Values not used in calculating the average melting point
-90.00	PHYSPROP[1]

1. clearly out of range JCB

1,3-dibromopropane C3H6Br2[3, 31, 61, 64]

Compound Data

Melting point	**-34.05 °C**	**239.10 K**			
CSID	7710	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	201.8877	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.93 g/cm^3
SMILES	BrCCCBr				
STD InChIKey	VEFLKXRACNJHOV-UHFFFAOYAK				

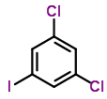
Melting Points

mp °C	source
-34.00	Alfa Aesar
-34.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-34.00	Oxford University MSDS
-34.20	PHYSPROP

1,3-dichloro-5-iodobenzene C6H3Cl2I[2, 3]

Compound Data

Melting point	**56.50 °C**	**329.65 K**			
CSID	68896	**H bond acceptors**	0	**Rule of 5 violations**	0



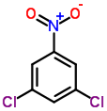
Molecular weight	272.8985	**H bond donors**	0	**ACD/LogP**	3.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.02 g/cm^3
SMILES	Ic1cc(Cl)cc(Cl)c1				
STD InChIKey	AATPRMRVLQZEHB-UHFFFAOYAC				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
57.00	Alfa Aesar

1,3-dichloro-5-nitrobenzene C6H3Cl2NO2[3, 64]

Compound Data



Melting point	**64.70 °C**	**337.85 K**			
CSID	11567	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.9995	**H bond donors**	0	**ACD/LogP**	3.34
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3
SMILES	Clc1cc([N+]([O-])=O)cc(Cl)c1				
STD InChIKey	RNABGKOKSBUFHW-UHFFFAOYAF				

Melting Points

mp °C	source
64.00	Alfa Aesar
65.40	PHYSPROP

1,3-dichloro-5,5-dimethylhydantoin C5H6Cl2N2O2[3, 61, 64]

Compound Data

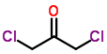
Melting point	**133.00 °C**	**406.15 K**			
CSID	8057	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	197.0193	**H bond donors**	0	**ACD/LogP**	1.35
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.58 g/cm^3
SMILES	O=C1N(Cl)C(=O)N(Cl)C1(C)C				
STD InChIKey	KEQGZUUPPQEDPF-UHFFFAOYAB				

Melting Points

mp °C	source
132.00	Alfa Aesar
135.00	Oxford University MSDS
132.00	PHYSPROP

1,3-dichloroacetone C3H4Cl2O[3, 64]

Compound Data



Melting point	**44.50 °C**	**317.65 K**			
CSID	21106513	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	126.9693	**H bond donors**	0	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.30 g/cm^3
SMILES	ClCC(=O)CCl				
STD InChIKey	SUNMBRGCANLOEG-UHFFFAOYAE				

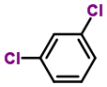
Melting Points

mp °C	source
44.00	Alfa Aesar
45.00	PHYSPROP

1,3-dichlorobenzene C6H4Cl2[3, 31, 61, 64]

Compound Data

Melting point	**-24.90 °C**	**248.25 K**	



CSID	13857694	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	147.002	**H bond donors**	0	**ACD/LogP**	3.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.30 g/cm^3
SMILES	Clc1cccc(Cl)c1				
STD InChIKey	ZPQOPVIELGIULI-UHFFFAOYAZ				

Melting Points

mp °C	source
-25.00	Alfa Aesar
-25.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-24.80	Oxford University MSDS
-24.80	PHYSPROP

1,3-dichloropropane C3H6Cl2[31, 64]

Compound Data

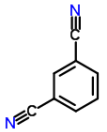
Melting point	**-99.75 °C**	**173.40 K**			
CSID	8543	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.9857	**H bond donors**	0	**ACD/LogP**	2.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.12 g/cm^3
SMILES	ClCCCCl				
STD InChIKey	YHRUOJUYPBUZOS-UHFFFAOYAZ				

Melting Points

mp °C	source
-100.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-99.50	PHYSPROP

1,3-dicyanobenzene C8H4N2[2, 3, 64]

Compound Data



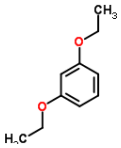
Melting point	**161.33 °C**	**434.48 K**			
CSID	11773	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.1308	**H bond donors**	0	**ACD/LogP**	0.82
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	N#Cc1cccc(C#N)c1				
STD InChIKey	LAQPNDIUHRHNCV-UHFFFAOYAQ				

Melting Points

mp °C	source
161.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
161.00	Alfa Aesar
162.00	PHYSPROP

1,3-diethoxybenzene C10H14O2[3, 64]

Compound Data



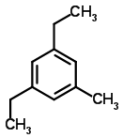
Melting point	**11.70 °C**	**284.85 K**			
CSID	67462	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	166.217	**H bond donors**	0	**ACD/LogP**	2.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.97 g/cm^3
SMILES	O(c1cccc(OCC)c1)CC				
STD InChIKey	MKGFYMKFBCWNCP-UHFFFAOYAG				

Melting Points

mp °C	source
11.00	Alfa Aesar
12.40	PHYSPROP

1,3-diethyl-5-methylbenzene C11H16[4, 64]

Compound Data



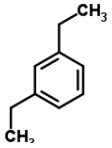
Melting point	**-74.05 °C**	**199.10 K**			
CSID	15468	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	148.2447	**H bond donors**	0	**ACD/LogP**	4.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.86 g/cm^3
SMILES	c1c(cc(cc1CC)CC)C				
STD InChIKey	HILAULICMJUOLK-UHFFFAOYAE				

Melting Points

mp °C	source
-74.00	American Petroleum Institute. Research Project 44; Selected ...
-74.10	PHYSPROP

1,3-diethylbenzene C10H14[4, 64]

Compound Data



Melting point	**-83.95 °C**	**189.20 K**			
CSID	8531	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.86 g/cm^3
SMILES	c1ccc(cc1CC)CC				
STD InChIKey	AFZZYIJIWUTJFO-UHFFFAOYAI				

Melting Points

mp °C	source
-84.00	American Petroleum Institute. Research Project 44; Selected ...
-83.90	PHYSPROP

1,3-diiodobenzene C6H4I2[3, 7, 64]

Compound Data

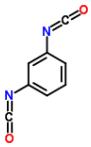
Melting point	**37.80 °C**	**310.95 K**			
CSID	21168837	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	329.9049	**H bond donors**	0	**ACD/LogP**	3.83
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.47 g/cm^3
SMILES	Ic1cccc(I)c1				
STD InChIKey	SFPQFQUXAJOWNF-UHFFFAOYAA				

Melting Points

mp °C	source
36.00	Alfa Aesar
37.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
40.40	PHYSPROP

1,3-diisocyanatobenzene C8H4N2O2[3, 64]

Compound Data



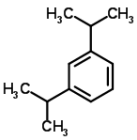
Melting point	**49.00 °C**	**322.15 K**			
CSID	29002	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	160.1296	**H bond donors**	0	**ACD/LogP**	3.01
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=C=N/c1cccc(\N=C=O)c1				
STD InChIKey	VGHSXKTVMPXHNG-UHFFFAOYAI				

Melting Points

mp °C	source
48.00	Alfa Aesar
50.00	PHYSPROP

1,3-diisopropylbenzene C12H18[2, 3, 64]

Compound Data



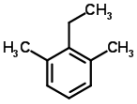
Melting point	**-63.03 °C**	**210.12 K**			
CSID	7170	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	162.2713	**H bond donors**	0	**ACD/LogP**	4.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.85 g/cm^3
SMILES	c1ccc(cc1C(C)C)C(C)C				
STD InChIKey	UNEATYXSUBPPKP-UHFFFAOYAQ				

Melting Points

mp °C	source
-63.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-63.00	Alfa Aesar
-63.10	PHYSPROP

1,3-dimethyl-2-ethylbenzene C10H14[4, 64]

Compound Data



Melting point	**-16.10 °C**	**257.05 K**			
CSID	16887	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1(cccc(c1CC)C)C				
STD InChIKey	CHIKRULMSSADAF-UHFFFAOYAK				

Melting Points

mp °C	source
-16.00	American Petroleum Institute. Research Project 44; Selected ...
-16.20	PHYSPROP

1,3-dimethyl-2-imidazolidinone C5H10N2O[3, 64]

Compound Data

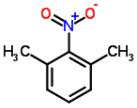
Melting point	**8.10 °C**	**281.25 K**			
CSID	6409	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	114.1457	**H bond donors**	0	**ACD/LogP**	0.55
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.06 g/cm^3
SMILES	CN1CCN(C1=O)C				
STD InChIKey	CYSGHNMQYZDMIA-UHFFFAOYAB				

Melting Points

mp °C	source
8.00	Alfa Aesar
8.20	PHYSPROP

1,3-dimethyl-2-nitrobenzene C8H9NO2[2, 3, 61, 64]

Compound Data

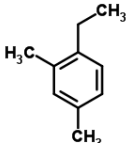


Melting point	**15.25 °C**	**288.40 K**			
CSID	6420	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	O=[N+]([O-])c1c(cccc1C)C				
STD InChIKey	HDFQKJQEWGVKCQ-UHFFFAOYAQ				

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
15.00	Alfa Aesar
15.00	Oxford University MSDS
15.00	PHYSPROP

1,3-dimethyl-4-ethylbenzene C10H14[4, 64]



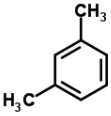
Compound Data

Melting point	**-62.95 °C**	**210.20 K**			
CSID	12829	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1cc(cc(c1CC)C)C				
STD InChIKey	MEMBJMDZWKVOTB-UHFFFAOYAK				

Melting Points

mp °C	source
-63.00	American Petroleum Institute. Research Project 44; Selected ...
-62.90	PHYSPROP

1,3-dimethylbenzene C8H10[3, 4, 64]



Compound Data

Melting point	**-47.60 °C**	**225.55 K**			
CSID	7641	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.165	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	Cc1cccc(c1)C				
STD InChIKey	IVSZLXZYQVIEFR-UHFFFAOYAX				

Melting Points

mp °C	source
-47.00	Alfa Aesar
-48.00	American Petroleum Institute. Research Project 44; Selected ...
-47.80	PHYSPROP

1,3-dimethyluracil C6H8N2O2[3, 64]

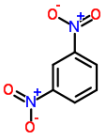
Compound Data

Melting point	**120.50 °C**	**393.65 K**			
CSID	63310	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	140.1399	**H bond donors**	0	**ACD/LogP**	0.40
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.22 g/cm^3
SMILES	O=C1N(C(=O)\C=C/N1C)C				
STD InChIKey	JSDBKAHWADVXFU-UHFFFAOYAJ				

Melting Points

mp °C	source
121.00	Alfa Aesar
120.00	PHYSPROP

1,3-dinitrobenzene C6H4N2O4[2, 3, 61, 64]



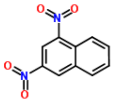
Compound Data

Melting point	**89.25 °C**	**362.40 K**			
CSID	7172	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	168.11	**H bond donors**	0	**ACD/LogP**	1.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.49 g/cm^3
SMILES	c1cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	WDCYWAQPCXBPJA-UHFFFAOYAZ				

Melting Points

mp °C	source
89.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
89.00	Alfa Aesar
89.00	Oxford University MSDS
90.00	PHYSPROP

1,3-dinitronaphthalene C10H6N2O4[61, 64]



Compound Data

Melting point	**147.50 °C**	**420.65 K**			
CSID	11325	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	218.1656	**H bond donors**	0	**ACD/LogP**	2.77
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.48 g/cm^3
SMILES	c1ccc2c(c1)cc(cc2N(=O)=O)N(=O)=O				
STD InChIKey	ULALSFRIGPMWRS-UHFFFAOYAZ				

Melting Points

mp °C	source
147.00	Oxford University MSDS
148.00	PHYSPROP

1,3-dioxane C4H8O2[61, 64]

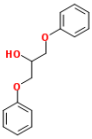
Compound Data

Melting point	**-43.50 °C**	**229.65 K**			
CSID	10018	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	0	**ACD/LogP**	-0.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.99 g/cm^3
SMILES	O1CCCOC1				
STD InChIKey	VDFVNEFVBPFDSB-UHFFFAOYAD				

Melting Points

mp °C	source
-42.00	Oxford University MSDS
-45.00	PHYSPROP

1,3-diphenoxy-2-propanol C15H16O3[3, 64]



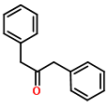
Compound Data

Melting point	**81.75 °C**	**354.90 K**			
CSID	11641	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	244.2857	**H bond donors**	1	**ACD/LogP**	3.07
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.15 g/cm^3
SMILES	O(c1ccccc1)CC(O)COc2ccccc2				
STD InChIKey	NKCVHIPHZCIEFC-UHFFFAOYAO				

Melting Points

mp °C	source
82.00	Alfa Aesar
81.50	PHYSPROP

1,3-diphenylacetone C15H14O[2, 3, 61, 64]



Compound Data

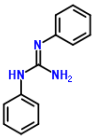
Melting point	**33.50 °C**	**306.65 K**			
CSID	21105887	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	210.2711	**H bond donors**	0	**ACD/LogP**	2.99
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.07 g/cm^3
SMILES	O=C(Cc1ccccc1)Cc2ccccc2				
STD InChIKey	YFKBXYGUSOXJGS-UHFFFAOYAS				

Melting Points

mp °C	source
33.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
34.00	Alfa Aesar
32.00	Oxford University MSDS
35.00	PHYSPROP

1,3-diphenylguanidine C13H13N3[3, 64]

Compound Data



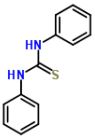
Melting point	**149.50 °C**	**422.65 K**			
CSID	7313	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	211.2624	**H bond donors**	3	**ACD/LogP**	2.85
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.10 g/cm^3
SMILES	N(=C(/Nc1ccccc1)N)\c2ccccc2				
STD InChIKey	OWRCNXZUPFZXOS-UHFFFAOYAB				

Melting Points

mp °C	source
149.00	Alfa Aesar
150.00	PHYSPROP

1,3-diphenylthiourea C13H12N2S[3, 61, 64]

Compound Data



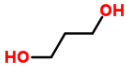
Melting point	**153.50 °C**	**426.65 K**			
CSID	610932	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	228.3128	**H bond donors**	2	**ACD/LogP**	2.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	S=C(Nc1ccccc1)Nc2ccccc2				
STD InChIKey	FCSHMCFRCYZTRQ-UHFFFAOYAC				

Melting Points

mp °C	source
152.00	Alfa Aesar
154.00	Oxford University MSDS
154.50	PHYSPROP

1,3-propanediol C3H8O2[2, 3, 64]

Compound Data



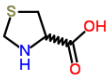
Melting point	**-26.57 °C**	**246.58 K**			
CSID	13839553	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	76.0944	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.04 g/cm^3
SMILES	C(CO)CO				
STD InChIKey	YPFDHNVEDLHUCE-UHFFFAOYAS				

Melting Points

mp °C	source
-27.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-26.00	Alfa Aesar
-26.70	PHYSPROP

1,3-thiazolidine-4-carboxylic acid C4H7NO2S[61, 64]

Compound Data



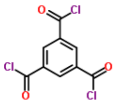
Melting point	**195.75 °C**	**468.90 K**			
CSID	9546	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	133.1689	**H bond donors**	2	**ACD/LogP**	-0.39
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.38 g/cm^3
SMILES	O=C(O)C1NCSC1				
STD InChIKey	DZLNHFMRPBPULJ-UHFFFAOYAN				

Melting Points

mp °C	source
195.00	Oxford University MSDS
196.50	PHYSPROP

1,3,5-benzenetricarbonyl chloride C9H3Cl3O3[3, 64]

Compound Data



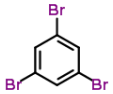
Melting point	**36.15 °C**	**309.30 K**			
CSID	70514	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	265.4773	**H bond donors**	0	**ACD/LogP**	3.02
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.57 g/cm^3
SMILES	O=C(Cl)c1cc(cc(C(Cl)=O)c1)C(Cl)=O				
STD InChIKey	UWCPYKQBIPYOLX-UHFFFAOYAM				

Melting Points

mp °C	source
36.00	Alfa Aesar
36.30	PHYSPROP

1,3,5-tribromobenzene C6H3Br3[2, 3, 64, 70]

Compound Data



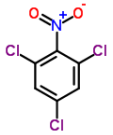
Melting point	**123.45 °C**	**396.60 K**			
CSID	11776	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	314.8	**H bond donors**	0	**ACD/LogP**	4.39
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.28 g/cm^3
SMILES	Brc1cc(Br)cc(Br)c1				
STD InChIKey	YWDUZLFWHVQCHY-UHFFFAOYAU				

Melting Points

mp °C	source
124.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
123.00	Alfa Aesar
122.80	PHYSPROP
124.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,3,5-trichloro-2-nitrobenzene C6H2Cl3NO2[3, 61, 64]

Compound Data



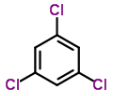
Melting point	**71.67 °C**	**344.82 K**			
CSID	27183	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.4446	**H bond donors**	0	**ACD/LogP**	3.41
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.65 g/cm^3
SMILES	O=[N+]([O-])c1c(Cl)cc(Cl)cc1Cl				
STD InChIKey	AEBJDOTVYMITIA-UHFFFAOYAF				

Melting Points

mp °C	source
71.00	Alfa Aesar
72.00	Oxford University MSDS
72.00	PHYSPROP

1,3,5-trichlorobenzene C6H3Cl3[2, 3, 44, 64, 70]

Compound Data



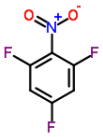
Melting point	**64.18 °C**	**337.33 K**			
CSID	7662	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	181.447	**H bond donors**	0	**ACD/LogP**	4.04
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.45 g/cm^3
SMILES	Clc1cc(Cl)cc(Cl)c1				
STD InChIKey	XKEFYDZQGKAQCN-UHFFFAOYAQ				

Melting Points

mp °C	source
65.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
64.00	Alfa Aesar
63.40	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
63.50	PHYSPROP

65.00 Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,3,5-trifluoro-2-nitrobenzene C6H2F3NO2[3, 64]



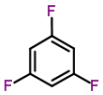
Compound Data

Melting point	**3.75 °C**	**276.90 K**			
CSID	60889	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	177.0808	**H bond donors**	0	**ACD/LogP**	1.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.55 g/cm^3
SMILES	O=[N+]([O-])c1c(F)cc(F)cc1F				
STD InChIKey	PWRFDGYYJWQIAB-UHFFFAOYAT				

Melting Points

mp °C	source
4.00	Alfa Aesar
3.50	PHYSPROP

1,3,5-trifluorobenzene C6H3F3[3, 64]



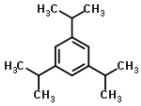
Compound Data

Melting point	**-5.75 °C**	**267.40 K**			
CSID	21111798	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	132.0832	**H bond donors**	0	**ACD/LogP**	2.49
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	Fc1cc(F)cc(F)c1				
STD InChIKey	JXUKFFRPLNTYIV-UHFFFAOYAT				

Melting Points

mp °C	source
-6.00	Alfa Aesar
-5.50	PHYSPROP

1,3,5-triisopropylbenzene C15H24[3, 64]



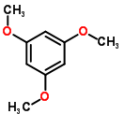
Compound Data

Melting point	**-7.20 °C**	**265.95 K**			
CSID	12329	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	204.3511	**H bond donors**	0	**ACD/LogP**	6.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.85 g/cm^3
SMILES	c1c(cc(cc1C(C)C)C(C)C)C(C)C				
STD InChIKey	VUMCUSHVMYIRMB-UHFFFAOYAA				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-7.40	PHYSPROP

1,3,5-trimethoxybenzene C9H12O3[2, 3, 64]



Compound Data

Melting point	**53.17 °C**	**326.32 K**			
CSID	21111723	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	168.1898	**H bond donors**	0	**ACD/LogP**	1.60
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.04 g/cm^3
SMILES	COc1cc(cc(OC)c1)OC				
STD InChIKey	LKUDPHPHKOZXCD-UHFFFAOYAM				

Melting Points

mp °C	source
53.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
52.00	Alfa Aesar
54.50	PHYSPROP

1,3,5-trimethylcyanuric acid $C_6H_9N_3O_3$[47, 64]

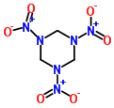
Compound Data

Melting point	**176.18 °C**	**449.32 K**			
CSID	12670	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	171.154	**H bond donors**	0	**ACD/LogP**	-2.92
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.32 g/cm^3
SMILES	O=C1N(C(=O)N(C(=O)N1C)C)C				
STD InChIKey	AHWDQDMGFXRVFB-UHFFFAOYAW				

Melting Points

mp °C	source
175.85	IUCr
176.50	PHYSPROP

1,3,5-trinitro-1,3,5-triazinane $C_3H_6N_6O_6$[61, 64]



Compound Data

Melting point	**205.25 °C**	**478.40 K**			
CSID	8177	**H bond acceptors**	12	**Rule of 5 violations**	1
Molecular weight	222.1163	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.90 g/cm^3
SMILES	C1N(CN(CN1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	XTFIVUDBNACUBN-UHFFFAOYAY				

Melting Points

mp °C	source
205.00	Oxford University MSDS
205.50	PHYSPROP

1,3,5-trioxane $C_3H_6O_3$[3, 64]

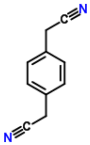
Compound Data

Melting point	**60.60 °C**	**333.75 K**			
CSID	7790	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	90.0779	**H bond donors**	0	**ACD/LogP**	-0.62
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	O1COCOC1				
STD InChIKey	BGJSXRVXTHVRSN-UHFFFAOYAW				

Melting Points

mp °C	source
61.00	Alfa Aesar
60.20	PHYSPROP

1,4-benzenediacetonitrile $C_{10}H_8N_2$[2, 3, 48]



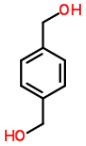
Compound Data

Melting point	**95.67 °C**	**368.82 K**			
CSID	62536	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.1839	**H bond donors**	0	**ACD/LogP**	0.68
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.10 g/cm^3
SMILES	N#CCc1ccc(cc1)CC#N				
STD InChIKey	FUQCKESKNZBNOG-UHFFFAOYAC				

Melting Points

mp °C	source
95.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
96.00	Alfa Aesar
96.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

1,4-benzenedimethanol $C_8H_{10}O_2$[2, 3, 64]



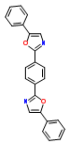
Compound Data

Melting point	**118.17 °C**	**391.32 K**			
CSID	11022	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	2	**ACD/LogP**	-0.15
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	OCc1ccc(cc1)CO				
STD InChIKey	BWVAOONFBYYRHY-UHFFFAOYAM				

Melting Points

mp °C	source
118.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
119.00	Alfa Aesar
117.50	PHYSPROP

1,4-bis(5-phenyloxazol-2-yl)benzene $C_{24}H_{16}N_2O_2$[3, 64]



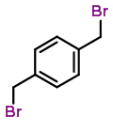
Compound Data

Melting point	**243.50 °C**	**516.65 K**			
CSID	14960	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	364.396	**H bond donors**	0	**ACD/LogP**	6.45
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	n1cc(oc1c4ccc(c2ncc(o2)c3ccccc3)cc4)c5ccccc5				
STD InChIKey	MASVCBBIUQRUKL-UHFFFAOYAO				

Melting Points

mp °C	source
242.00	Alfa Aesar
245.00	PHYSPROP

1,4-bis(bromomethyl)benzene $C_8H_8Br_2$[48, 64]



Compound Data

Melting point	**143.25 °C**	**416.40 K**			
CSID	21125563	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	263.9571	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.78 g/cm^3
SMILES	BrCc1ccc(CBr)cc1				
STD InChIKey	RBZMSGOBSOCYHR-UHFFFAOYAL				

Melting Points

mp °C	source
142.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
144.50	PHYSPROP

1,4-cyclohexadiene C_6H_8[3, 64]

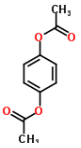
Compound Data

Melting point	**-49.10 °C**	**224.05 K**			
CSID	11838	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	80.1277	**H bond donors**	0	**ACD/LogP**	2.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.86 g/cm^3
SMILES	C\1=C\C/C=C\C/1				
STD InChIKey	UVJHQYIOXKWHFD-UHFFFAOYAM				

Melting Points

mp °C	source
-49.00	Alfa Aesar
-49.20	PHYSPROP

1,4-diacetoxybenzene $C_{10}H_{10}O_4$[3, 7, 64]



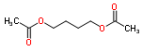
Compound Data

Melting point	**123.17 °C**	**396.32 K**			
CSID	64166	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	0.98
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(Oc1ccc(OC(=O)C)cc1)C				
STD InChIKey	AKOGNYJNGMLDOA-UHFFFAOYAQ				

Melting Points

mp °C	source
121.00	Alfa Aesar
125.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
123.50	PHYSPROP

1,4-diacetoxybutane C8H14O4[3, 64]



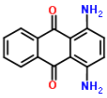
Compound Data

Melting point	**12.50 °C**	**285.65 K**			
CSID	62618	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1944	**H bond donors**	0	**ACD/LogP**	0.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.04 g/cm^3
SMILES	O=C(OCCCCOC(=O)C)C				
STD InChIKey	XUKSWKGOQKREON-UHFFFAOYAS				

Melting Points

mp °C	source
13.00	Alfa Aesar
12.00	PHYSPROP

1,4-diaminoanthraquinone C14H10N2O2[3, 64]



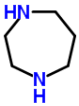
Compound Data

Melting point	**265.50 °C**	**538.65 K**			
CSID	29150	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	238.2414	**H bond donors**	4	**ACD/LogP**	2.98
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.46 g/cm^3
SMILES	O=C2c1ccccc1C(=O)c3c2c(ccc3N)N				
STD InChIKey	FBMQNRKSAWNXBT-UHFFFAOYAJ				

Melting Points

mp °C	source
263.00	Alfa Aesar
268.00	PHYSPROP

1,4-diazepane C5H12N2[3, 64]



Compound Data

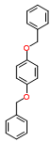
Melting point	**42.25 °C**	**315.40 K**			
CSID	61471	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1622	**H bond donors**	2	**ACD/LogP**	-0.48
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.86 g/cm^3
SMILES	N1CCCNCC1				
STD InChIKey	FQUYSHZXSKYCSY-UHFFFAOYAL				

Melting Points

mp °C	source
41.00	Alfa Aesar
43.50	PHYSPROP

1,4-dibenzyloxybenzene C20H18O2[3, 48]

Compound Data



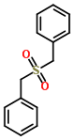
Melting point	**127.50 °C**	**400.65 K**			
CSID	62525	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	290.3557	**H bond donors**	0	**ACD/LogP**	5.41
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.12 g/cm^3
SMILES	O(c2ccc(OCc1ccccc1)cc2)Cc3ccccc3				
STD InChIKey	DYULYMCXVSRUPB-UHFFFAOYAS				

Melting Points

mp °C	source
127.00	Alfa Aesar
128.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

1,4-dibenzyloxybenzene C14H14O2S[3, 64]

Compound Data



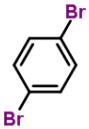
Melting point	**151.50 °C**	**424.65 K**			
CSID	62493	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	246.3248	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.21 g/cm^3
SMILES	O=S(=O)(Cc1ccccc1)Cc2ccccc2				
STD InChIKey	AWHNUHMUCGRKRA-UHFFFAOYAM				

Melting Points

mp °C	source
151.00	Alfa Aesar
152.00	PHYSPROP

1,4-dibromobenzene C6H4Br2[2, 3, 44, 61, 64, 70]

Compound Data



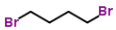
Melting point	**87.60 °C**	**360.75 K**			
CSID	13868640	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	235.904	**H bond donors**	0	**ACD/LogP**	3.79
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.94 g/cm^3
SMILES	Brc1ccc(Br)cc1				
STD InChIKey	SWJPEBQEEAHIGZ-UHFFFAOYAE				

Melting Points

mp °C	source
88.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
88.00	Alfa Aesar
87.30	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
88.00	Oxford University MSDS
87.30	PHYSPROP
87.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,4-dibromobutane C4H8Br2[3, 31, 61, 64]

Compound Data

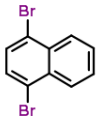


Melting point	**-18.38 °C**	**254.77 K**			
CSID	7765	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	215.9143	**H bond donors**	0	**ACD/LogP**	2.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.78 g/cm^3
SMILES	BrCCCCBr				
STD InChIKey	ULTHEAFYOOPTTB-UHFFFAOYAB				

Melting Points

mp °C	source
-20.00	Alfa Aesar
-17.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-20.00	Oxford University MSDS
-16.50	PHYSPROP

1,4-dibromonaphthalene $C_{10}H_6Br_2$[3, 64]



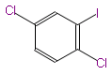
Compound Data

Melting point	**82.00 °C**	**355.15 K**			
CSID	59892	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	285.9626	**H bond donors**	0	**ACD/LogP**	5.02
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.83 g/cm^3
SMILES	Brc2c1ccccc1c(Br)cc2				
STD InChIKey	IBGUDZMIAZLJNY-UHFFFAOYAE				

Melting Points

mp °C	source
81.00	Alfa Aesar
83.00	PHYSPROP

1,4-dichloro-2-iodobenzene $C_6H_3Cl_2I$[2, 3, 64]



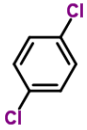
Compound Data

Melting point	**21.33 °C**	**294.48 K**			
CSID	21171496	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	272.8985	**H bond donors**	0	**ACD/LogP**	4.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.02 g/cm^3
SMILES	Clc1ccc(Cl)c(I)c1				
STD InChIKey	SBHVNORGKIPGCL-UHFFFAOYAS				

Melting Points

mp °C	source
21.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
21.00	Alfa Aesar
22.00	PHYSPROP

1,4-dichlorobenzene $C_6H_4Cl_2$[3, 31, 61, 64, 70, 70, 70]



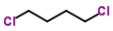
Compound Data

Melting point	**53.01 °C**	**326.16 K**			
CSID	13866817	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	147.002	**H bond donors**	0	**ACD/LogP**	3.34
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.30 g/cm^3
SMILES	Clc1ccc(Cl)cc1				
STD InChIKey	OCJBOOLMMGQPQU-UHFFFAOYAL				

Melting Points

mp °C	source
54.00	Alfa Aesar
53.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
53.00	Oxford University MSDS
52.09	PHYSPROP
53.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
53.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
53.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

1,4-dichlorobutane $C_4H_8Cl_2$[3, 31, 61, 64]



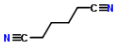
Compound Data

Melting point	**-37.58 °C**	**235.57 K**			
CSID	21106032	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	127.0123	**H bond donors**	0	**ACD/LogP**	2.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	ClCCCCCl				
STD InChIKey	KJDRSWPQXHESDQ-UHFFFAOYAC				

Melting Points

mp °C	source
-38.00	Alfa Aesar
-37.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-38.00	Oxford University MSDS
-37.30	PHYSPROP

1,4-dicyanobutane C6H8N2[2, 3, 64]



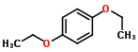
Compound Data

Melting point	**1.67 °C**	**274.82 K**			
CSID	13876621	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.94 g/cm^3
SMILES	N#CCCCCC#N				
STD InChIKey	BTGRAWJCKBQKAO-UHFFFAOYAW				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
2.00	Alfa Aesar
1.00	PHYSPROP

1,4-diethoxybenzene C10H14O2[3, 7, 64]



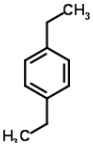
Compound Data

Melting point	**71.33 °C**	**344.48 K**			
CSID	21111774	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	166.217	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.97 g/cm^3
SMILES	CCOc1ccc(cc1)OCC				
STD InChIKey	VWGNFIQXBYRDCH-UHFFFAOYAX				

Melting Points

mp °C	source
70.00	Alfa Aesar
72.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
72.00	PHYSPROP

1,4-diethylbenzene C10H14[3, 4, 64]



Compound Data

Melting point	**-42.94 °C**	**230.21 K**			
CSID	7448	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.86 g/cm^3
SMILES	c1cc(ccc1CC)CC				
STD InChIKey	DSNHSQKRULAAEI-UHFFFAOYAQ				

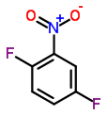
Melting Points

mp °C	source
-43.00	Alfa Aesar
-43.00	American Petroleum Institute. Research Project 44; Selected ...
-42.83	PHYSPROP

1,4-difluoro-2-nitrobenzene C6H3F2NO2[3, 64]

Compound Data

Melting point	**-11.85 °C**	**261.30 K**			
CSID	61086	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	159.0903	**H bond donors**	0	**ACD/LogP**	1.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.45 g/cm^3



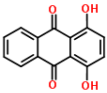
SMILES	O=[N+]([O-])c1cc(F)ccc1F
STD InChIKey	XNJAYQHWXYJBBD-UHFFFAOYAS

Melting Points

mp °C	source
-12.00	Alfa Aesar
-11.70	PHYSPROP

1,4-dihydroxyanthraquinone C14H8O4[3, 64]

Compound Data



Melting point	**198.50 °C**	**471.65 K**			
CSID	6433	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	240.2109	**H bond donors**	2	**ACD/LogP**	4.46
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.54 g/cm^3
SMILES	O=C2c1ccccc1C(=O)c3c2c(O)ccc3O				
STD InChIKey	GUEIZVNYDFNHJU-UHFFFAOYAX				

Melting Points

mp °C	source
197.00	Alfa Aesar
200.00	PHYSPROP

1,4-diiodobenzene C6H4I2[2, 3, 64]

Compound Data

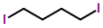
Melting point	**130.83 °C**	**403.98 K**			
CSID	11708	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	329.9049	**H bond donors**	0	**ACD/LogP**	4.11
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.47 g/cm^3
SMILES	Ic1ccc(I)cc1				
STD InChIKey	LFMWZTSOMGDDJU-UHFFFAOYAW				

Melting Points

mp °C	source
131.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
130.00	Alfa Aesar
131.50	PHYSPROP

1,4-diiodobutane C4H8I2[3, 64]

Compound Data



Melting point	**5.90 °C**	**279.05 K**			
CSID	11832	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	309.9153	**H bond donors**	0	**ACD/LogP**	3.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	2.34 g/cm^3
SMILES	ICCCCI				
STD InChIKey	ROUYUBHVBIKMQO-UHFFFAOYAC				

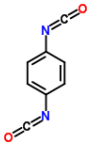
Melting Points

mp °C	source
6.00	Alfa Aesar
5.80	PHYSPROP

1,4-diisocyanatobenzene C8H4N2O2[61, 64]

Compound Data

Melting point	**95.75 °C**	**368.90 K**



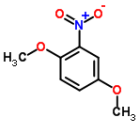
CSID	54970	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	160.1296	**H bond donors**	0	**ACD/LogP**	2.85
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=C=N/c1ccc(/N=C=O)cc1				
STD InChIKey	ALQLPWJFHRMHIU-UHFFFAOYAR				

Melting Points

mp °C	source
94.00	Oxford University MSDS
97.50	PHYSPROP

1,4-dimethoxy-2-nitrobenzene C8H9NO4[7, 64]

Compound Data



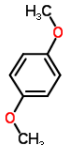
Melting point	**71.75 °C**	**344.90 K**			
CSID	60006	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	183.1614	**H bond donors**	0	**ACD/LogP**	2.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	[O-][N+](=O)c1cc(OC)ccc1OC				
STD InChIKey	UPTOWXNJLZJTGD-UHFFFAOYAH				

Melting Points

mp °C	source
71.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
72.50	PHYSPROP

1,4-dimethoxybenzene C8H10O2[2, 3, 61, 64]

Compound Data



Melting point	**58.25 °C**	**331.40 K**			
CSID	21105878	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	0	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.00 g/cm^3
SMILES	COc1ccc(OC)cc1				
STD InChIKey	OHBQPCCCRFSCAX-UHFFFAOYAX				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
56.00	Alfa Aesar
58.00	Oxford University MSDS
59.00	PHYSPROP

1,4-dimethylbenzene C8H10[3, 4, 64]

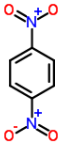
Compound Data

Melting point	**12.75 °C**	**285.90 K**			
CSID	7521	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.165	**H bond donors**	0	**ACD/LogP**	3.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	Cc1ccc(cc1)C				
STD InChIKey	URLKBWYHVLBVBO-UHFFFAOYAE				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.00	American Petroleum Institute. Research Project 44; Selected ...
13.25	PHYSPROP

1,4-dinitrobenzene C6H4N2O4[2, 3, 64]



Compound Data

Melting point	**173.67 °C**	**446.82 K**			
CSID	7211	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	168.107	**H bond donors**	0	**ACD/LogP**	1.37
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.49 g/cm^3
SMILES	O=[N+]([O-])c1ccc([N+]([O-])=O)cc1				
STD InChIKey	FYFDQJRXFWGIBS-UHFFFAOYAB				

Melting Points

mp °C	source
173.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
174.00	Alfa Aesar
174.00	PHYSPROP

1,4-dioxane C4H8O2[3, 61, 64]

Compound Data

Melting point	**11.87 °C**	**285.02 K**			
CSID	29015	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	0	**ACD/LogP**	-0.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.99 g/cm^3
SMILES	O1CCOCC1				
STD InChIKey	RYHBNJHYFVUHQT-UHFFFAOYAN				

Melting Points

mp °C	source
12.00	Alfa Aesar
11.80	Oxford University MSDS
11.80	PHYSPROP

1,4-dithiane C4H8S2[61, 64]

Compound Data

Melting point	**111.65 °C**	**384.80 K**			
CSID	10020	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.2363	**H bond donors**	0	**ACD/LogP**	1.12
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	S1CCSCC1				
STD InChIKey	LOZWAPSEEHRYPG-UHFFFAOYAR				

Melting Points

mp °C	source
111.00	Oxford University MSDS
112.30	PHYSPROP

1,4-pentadiene C5H8[4, 61, 64]

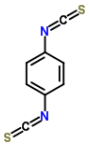
Compound Data

Melting point	**-148.27 °C**	**124.88 K**			
CSID	11099	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	68.117	**H bond donors**	0	**ACD/LogP**	2.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.67 g/cm^3
SMILES	C=C\C\C=C				
STD InChIKey	QYZLKGVUSQXAMU-UHFFFAOYAD				

Melting Points

mp °C	source
-148.00	American Petroleum Institute. Research Project 44; Selected ...
-148.00	Oxford University MSDS
-148.80	PHYSPROP

1,4-phenylene diisothiocyanate C8H4N2S2[3, 64]



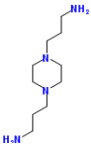
Compound Data

Melting point	**131.50 °C**	**404.65 K**			
CSID	18799	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	192.2608	**H bond donors**	0	**ACD/LogP**	4.16
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	S=C=N/c1ccc(/N=C=S)cc1				
STD InChIKey	OMWQUXGVXQELIX-UHFFFAOYAS				

Melting Points

mp °C	source
131.00	Alfa Aesar
132.00	PHYSPROP

1,4-piperazinedipropanamine C10H24N4[3, 64]



Compound Data

Melting point	**14.50 °C**	**287.65 K**			
CSID	73658	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	200.3244	**H bond donors**	4	**ACD/LogP**	-1.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.98 g/cm^3
SMILES	N1(CCN(CCCN)CC1)CCCN				
STD InChIKey	XUSNPFGLKGCWGN-UHFFFAOYAN				

Melting Points

mp °C	source
14.00	Alfa Aesar
15.00	PHYSPROP

1,5-dichloropentane C5H10Cl2[3, 31, 64]

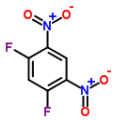
Compound Data

Melting point	**-72.60 °C**	**200.55 K**			
CSID	21106526	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	141.0389	**H bond donors**	0	**ACD/LogP**	2.78
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.05 g/cm^3
SMILES	ClCCCCCCl				
STD InChIKey	LBKDGROORAKTLC-UHFFFAOYAO				

Melting Points

mp °C	source
-72.00	Alfa Aesar
-73.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-72.80	PHYSPROP

1,5-difluoro-2,4-dinitrobenzene C6H2F2N2O4[3, 64]



Compound Data

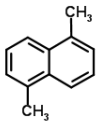
Melting point	**73.50 °C**	**346.65 K**			
CSID	60919	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	204.0879	**H bond donors**	0	**ACD/LogP**	0.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.68 g/cm^3
SMILES	O=[N+]([O-])c1cc(c(F)cc1F)[N+]([O-])=O				
STD InChIKey	VILFTWLXLYIEMV-UHFFFAOYAH				

Melting Points

mp °C	source
74.00	Alfa Aesar
73.00	PHYSPROP

1,5-dimethylnaphthalene C12H12[3, 64]

Compound Data



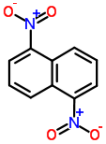
Melting point	**81.00 °C**	**354.15 K**			
CSID	10831	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	156.2237	**H bond donors**	0	**ACD/LogP**	4.37
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	c1ccc(c2cccc(c12)C)C				
STD InChIKey	SDDBCEWUYXVGCQ-UHFFFAOYAA				

Melting Points

mp °C	source
80.00	Alfa Aesar
82.00	PHYSPROP

1,5-dinitronaphthalene C10H6N2O4[3, 64]

Compound Data



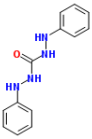
Melting point	**217.50 °C**	**490.65 K**			
CSID	11310	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	218.1656	**H bond donors**	0	**ACD/LogP**	2.58
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.48 g/cm^3
SMILES	[O-][N+](=O)c1cccc2c1cccc2[N+]([O-])=O				
STD InChIKey	ZUTCJXFCHHDFJS-UHFFFAOYAT				

Melting Points

mp °C	source
216.00	Alfa Aesar
219.00	PHYSPROP

1,5-diphenylcarbazide C13H14N4O[61, 64]

Compound Data



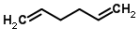
Melting point	**171.50 °C**	**444.65 K**			
CSID	8459	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	242.2765	**H bond donors**	4	**ACD/LogP**	2.24
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.29 g/cm^3
SMILES	O=C(NNc1ccccc1)NNc2ccccc2				
STD InChIKey	KSPIHGBHKVISFI-UHFFFAOYAZ				

Melting Points

mp °C	source
173.00	Oxford University MSDS
170.00	PHYSPROP

1,5-hexadiene C6H10[3, 4, 64]

Compound Data



Melting point	**-140.90 °C**	**132.25 K**			
CSID	11110	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.70 g/cm^3
SMILES	C=C\CC\C=C				
STD InChIKey	PYGSKMBEVAICCR-UHFFFAOYAB				

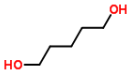
Melting Points

mp °C	source
-141.00	Alfa Aesar
-141.00	American Petroleum Institute. Research Project 44; Selected ...
-140.70	PHYSPROP

1,5-pentanediol C5H12O2[3, 64]

Compound Data

Melting point	**-17.00 °C**	**256.15 K**	



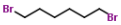
CSID	13839441	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	104.1476	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.98 g/cm^3
SMILES	C(CCO)CCO				
STD InChIKey	ALQSHHUCVQOPAS-UHFFFAOYAE				

Melting Points

mp °C	source
-16.00	Alfa Aesar
-18.00	PHYSPROP

1,6-dibromohexane C6H12Br2[3, 61, 64]

Compound Data



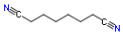
Melting point	**-0.77 °C**	**272.38 K**			
CSID	11862	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	243.9675	**H bond donors**	0	**ACD/LogP**	3.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.58 g/cm^3
SMILES	BrCCCCCCBr				
STD InChIKey	SGRHVVLXEBNBDV-UHFFFAOYAK				

Melting Points

mp °C	source
-2.00	Alfa Aesar
2.00	Oxford University MSDS
-2.30	PHYSPROP

1,6-dicyanohexane C8H12N2[2, 3, 64]

Compound Data



Melting point	**-3.17 °C**	**269.98 K**			
CSID	11879	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1943	**H bond donors**	0	**ACD/LogP**	0.48
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.92 g/cm^3
SMILES	N#CCCCCCCC#N				
STD InChIKey	BTNXBLUGMAMSSH-UHFFFAOYAE				

Melting Points

mp °C	source
-3.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-3.00	Alfa Aesar
-3.50	PHYSPROP

1,6-hexanediamine C6H16N2[3, 61, 64]

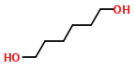
Compound Data

Melting point	**40.50 °C**	**313.65 K**			
CSID	13835579	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.2046	**H bond donors**	4	**ACD/LogP**	0.04
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	0.86 g/cm^3
SMILES	NCCCCCCN				
STD InChIKey	NAQMVNRVTILPCV-UHFFFAOYAS				

Melting Points

mp °C	source
41.00	Alfa Aesar
39.00	Oxford University MSDS
41.50	PHYSPROP

1,6-hexanediol C6H14O2[2, 3, 32, 64]



Compound Data

Melting point	**43.70 °C**	**316.85 K**			
CSID	13839416	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1742	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	0.96 g/cm^3
SMILES	OCCCCCCO				
STD InChIKey	XXMIOPMDWAUFGU-UHFFFAOYAU				

Melting Points

mp °C	source
45.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
42.00	Alfa Aesar
45.00	DrugBank
42.80	PHYSPROP

1,7-heptanediol C7H16O2[3, 64]

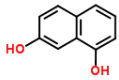
Compound Data

Melting point	**20.25 °C**	**293.40 K**			
CSID	11875	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	132.2007	**H bond donors**	2	**ACD/LogP**	0.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.95 g/cm^3
SMILES	OCCCCCCCO				
STD InChIKey	SXCBDZAEHILGLM-UHFFFAOYAS				

Melting Points

mp °C	source
18.00	Alfa Aesar
22.50	PHYSPROP

1,7-naphthalenediol C10H8O2[3, 64]



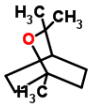
Compound Data

Melting point	**181.25 °C**	**454.40 K**			
CSID	61739	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.1693	**H bond donors**	2	**ACD/LogP**	1.94
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	Oc1c2c(ccc1)ccc(O)c2				
STD InChIKey	ZUVBIBLYOCVYJU-UHFFFAOYAO				

Melting Points

mp °C	source
182.00	Alfa Aesar
180.50	PHYSPROP

1,8-cineole C10H18O[3, 64]



Compound Data

Melting point	**1.25 °C**	**274.40 K**			
CSID	2656	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	154.2493	**H bond donors**	0	**ACD/LogP**	2.82
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.92 g/cm^3
SMILES	O2C1(CCC(CC1)C2(C)C)C				
STD InChIKey	WEEGYLXZBRQIMU-UHFFFAOYAY				

Melting Points

mp °C	source
1.00	Alfa Aesar
1.50	PHYSPROP

1,8-diaminonaphthalene C10H10N2[3, 64]

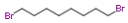
Compound Data

Melting point	**64.75 °C**	**337.90 K**			
CSID	61381	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1998	**H bond donors**	4	**ACD/LogP**	0.89
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	c1(cccc2cccc(N)c12)N				
STD InChIKey	YFOOEYJGMMJJLS-UHFFFAOYAU				

Melting Points

mp °C	source
63.00	Alfa Aesar
66.50	PHYSPROP

1,8-dibromooctane C8H16Br2[3, 61, 64]



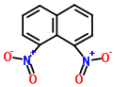
Compound Data

Melting point	**15.67 °C**	**288.82 K**			
CSID	70682	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	272.0206	**H bond donors**	0	**ACD/LogP**	4.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.46 g/cm^3
SMILES	BrCCCCCCCCBr				
STD InChIKey	DKEGCUDAFWNSSO-UHFFFAOYAR				

Melting Points

mp °C	source
16.00	Alfa Aesar
15.50	Oxford University MSDS
15.50	PHYSPROP

1,8-dinitronaphthalene C10H6N2O4[61, 64]



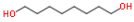
Compound Data

Melting point	**172.25 °C**	**445.40 K**			
CSID	11271	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	218.1656	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.48 g/cm^3
SMILES	[O-][N+](=O)c1cccc2cccc([N+]([O-])=O)c12				
STD InChIKey	AVCSMMMOCOTIHF-UHFFFAOYAR				

Melting Points

mp °C	source
171.50	Oxford University MSDS
173.00	PHYSPROP

1,8-octanediol C8H18O2[3, 64]



Compound Data

Melting point	**61.50 °C**	**334.65 K**			
CSID	62628	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	146.2273	**H bond donors**	2	**ACD/LogP**	0.99
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	0.94 g/cm^3
SMILES	OCCCCCCCCO				
STD InChIKey	OEIJHBUUFURJLI-UHFFFAOYAW				

Melting Points

mp °C	source
60.00	Alfa Aesar
63.00	PHYSPROP

1,9-nonanediol C9H20O2[3, 64]

Compound Data

Melting point	**46.40 °C**	**319.55 K**			
CSID	18685	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.2539	**H bond donors**	2	**ACD/LogP**	1.53
Phase 25 °C	solid	**Rotatable bonds**	10	**Predicted density**	0.93 g/cm^3
SMILES	OCCCCCCCCCCO				
STD InChIKey	ALVZNPYWJMLXKV-UHFFFAOYAQ				

Melting Points

mp °C	source
47.00	Alfa Aesar
45.80	PHYSPROP

10-undecen-1-ol C11H22O[3, 64]

Compound Data

Melting point	**-2.50 °C**	**270.65 K**			
CSID	7893	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2918	**H bond donors**	1	**ACD/LogP**	4.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	0.84 g/cm^3
SMILES	C=CCCCCCCCCCO				
STD InChIKey	GIEMHYCMBGELGY-UHFFFAOYAA				

Melting Points

mp °C	source
-3.00	Alfa Aesar
-2.00	PHYSPROP

10-undecenoic acid C11H20O2[3, 64]

Compound Data

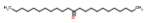
Melting point	**24.25 °C**	**297.40 K**			
CSID	10771160	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	184.2753	**H bond donors**	1	**ACD/LogP**	3.85
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.92 g/cm^3
SMILES	C=CCCCCCCCCC(=O)O				
STD InChIKey	FRPZMMHWLSIFAZ-UHFFFAOYAJ				

Melting Points

mp °C	source
24.00	Alfa Aesar
24.50	PHYSPROP

12-tricosanone C23H46O[3, 64]

Compound Data



Melting point	**68.60 °C**	**341.75 K**			
CSID	10426	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	338.6107	**H bond donors**	0	**ACD/LogP**	10.47
Phase 25 °C	solid	**Rotatable bonds**	20	**Predicted density**	0.83 g/cm^3
SMILES	O=C(CCCCCCCCCCC)CCCCCCCCCCC				
STD InChIKey	VARQGBHBYZTYLJ-UHFFFAOYAG				

Melting Points

mp °C	source
67.00	Alfa Aesar
70.20	PHYSPROP

14-heptacosanone C27H54O[3, 64]

Compound Data

Melting point	**77.75 °C**	**350.90 K**			
CSID	10490	**H bond acceptors**	1	**Rule of 5 violations**	1

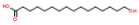
Molecular weight	394.7171	**H bond donors**	0	**ACD/LogP**	12.60
Phase 25 °C	solid	**Rotatable bonds**	24	**Predicted density**	0.84 g/cm^3
SMILES	O=C(CCCCCCCCCCCCCC)CCCCCCCCCCCCC				
STD InChIKey	VCZMOZVQLARCOE-UHFFFAOYAR				

Melting Points

mp °C	source
78.00	Alfa Aesar
77.50	PHYSPROP

16-hydroxyhexadecanoic acid C16H32O3[3, 64]

Compound Data



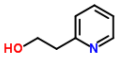
Melting point	**98.50 °C**	**371.65 K**			
CSID	10034	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	272.4235	**H bond donors**	2	**ACD/LogP**	5.15
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	0.96 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCCCCO				
STD InChIKey	UGAGPNKCDRTDHP-UHFFFAOYAB				

Melting Points

mp °C	source
99.00	Alfa Aesar
98.00	PHYSPROP

2-(2-hydroxyethyl)pyridine C7H9NO[3, 64]

Compound Data



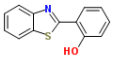
Melting point	**-7.90 °C**	**265.25 K**			
CSID	7392	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	123.1525	**H bond donors**	1	**ACD/LogP**	-0.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.09 g/cm^3
SMILES	OCCc1ncccc1				
STD InChIKey	BXGYBSJAZFGIPX-UHFFFAOYAP				

Melting Points

mp °C	source
-8.00	Alfa Aesar
-7.80	PHYSPROP

2-(2-hydroxyphenyl)benzothiazole C13H9NOS[3, 64]

Compound Data



Melting point	**131.50 °C**	**404.65 K**			
CSID	10181821	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	227.2817	**H bond donors**	1	**ACD/LogP**	4.53
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	Oc3ccccc3c1nc2ccccc2s1				
STD InChIKey	MVVGSPCXHRFDDR-UHFFFAOYAD				

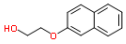
Melting Points

mp °C	source
132.00	Alfa Aesar
131.00	PHYSPROP

2-(2-naphthoxy)ethanol C12H12O2[3, 64]

Compound Data

Melting point	**75.35 °C**	**348.50 K**			
CSID	6864	**H bond acceptors**	2	**Rule of 5 violations**	0

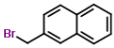


Molecular weight	188.2225	**H bond donors**	1	**ACD/LogP**	2.39
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.16 g/cm^3
SMILES	OCCOc2ccc1c(cccc1)c2				
STD InChIKey	BQPBZDSDFCDSAO-UHFFFAOYAT				

Melting Points

mp °C	source
74.00	Alfa Aesar
76.70	PHYSPROP

2-(bromomethyl)naphthalene C11H9Br[3, 64]



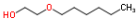
Compound Data

Melting point	**54.50 °C**	**327.65 K**			
CSID	63503	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	221.0932	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.44 g/cm^3
SMILES	BrCc2ccc1c(cccc1)c2				
STD InChIKey	RUHJZSZTSCSTCC-UHFFFAOYAS				

Melting Points

mp °C	source
53.00	Alfa Aesar
56.00	PHYSPROP

2-(hexyloxy)ethanol C8H18O2[3, 64]



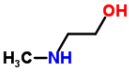
Compound Data

Melting point	**-43.55 °C**	**229.60 K**			
CSID	7878	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	146.2273	**H bond donors**	1	**ACD/LogP**	1.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.89 g/cm^3
SMILES	OCCOCCCCCC				
STD InChIKey	UPGSWASWQBLSKZ-UHFFFAOYAH				

Melting Points

mp °C	source
-42.00	Alfa Aesar
-45.10	PHYSPROP

2-(methylamino)ethanol C3H9NO[3, 61, 64]



Compound Data

Melting point	**-4.67 °C**	**268.48 K**			
CSID	13836021	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	75.1097	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.89 g/cm^3
SMILES	CNCCO				
STD InChIKey	OPKOKAMJFNKNAS-UHFFFAOYAK				

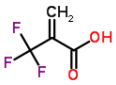
Melting Points

mp °C	source
-5.00	Alfa Aesar
-4.50	Oxford University MSDS
-4.50	PHYSPROP

2-(trifluoromethyl)acrylic acid C4H3F3O2[3, 64]

Compound Data

Melting point	**50.75 °C**	**323.90 K**



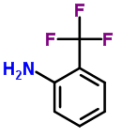
CSID	510851	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	140.0606	**H bond donors**	1	**ACD/LogP**	2.14
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	FC(F)(F)C(=C)\C(=O)O				
STD InChIKey	VLSRKCIBHNJFHA-UHFFFAOYAY				

Melting Points

mp °C	source
50.00	Alfa Aesar
51.50	PHYSPROP

2-(trifluoromethyl)aniline C7H6F3N[3, 38, 64, 72]

Compound Data



Melting point	**-31.00 °C**	**242.15 K**			
CSID	6656	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	161.1244	**H bond donors**	2	**ACD/LogP**	2.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	FC(F)(F)c1ccccc1N				
STD InChIKey	VBLXCTYLWZJBKA-UHFFFAOYAE				

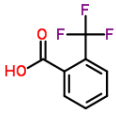
Melting Points

mp °C	source
-34.00	Alfa Aesar
-30.00	Fluoryx
-29.00	Sigma-Aldrich
	Values not used in calculating the average melting point
35.50	PHYSPROP[1]

1. out of range and index of refraction reported at 20C JCB

2-(trifluoromethyl)benzoic acid C8H5F3O2[3, 64]

Compound Data



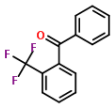
Melting point	**110.00 °C**	**383.15 K**			
CSID	9515	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	190.1193	**H bond donors**	1	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	FC(F)(F)c1ccccc1C(=O)O				
STD InChIKey	FBRJYBGLCHWYOE-UHFFFAOYAQ				

Melting Points

mp °C	source
109.00	Alfa Aesar
111.00	PHYSPROP

2-(trifluoromethyl)benzophenone C14H9F3O[3, 64]

Compound Data

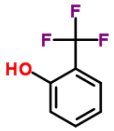


Melting point	**60.50 °C**	**333.65 K**			
CSID	62963	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	250.2159	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	FC(F)(F)c2ccccc2C(=O)c1ccccc1				
STD InChIKey	JXIWJBWMQXDALU-UHFFFAOYAU				

Melting Points

mp °C	source
60.00	Alfa Aesar
61.00	PHYSPROP

2-(trifluoromethyl)phenol C7H5F3O[3, 61, 64]



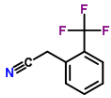
Compound Data

Melting point	**45.67 °C**	**318.82 K**			
CSID	61273	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.1092	**H bond donors**	1	**ACD/LogP**	2.67
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	FC(F)(F)c1ccccc1O				
STD InChIKey	ZOQOPXVJANRGJZ-UHFFFAOYAM				

Melting Points

mp °C	source
46.00	Alfa Aesar
45.50	Oxford University MSDS
45.50	PHYSPROP

2-(trifluoromethyl)phenylacetonitrile C9H6F3N[3, 64]



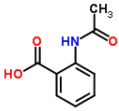
Compound Data

Melting point	**31.50 °C**	**304.65 K**			
CSID	68907	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	185.1458	**H bond donors**	0	**ACD/LogP**	2.02
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	FC(F)(F)c1ccccc1CC#N				
STD InChIKey	QXDCZSJGEUSERL-UHFFFAOYAD				

Melting Points

mp °C	source
30.00	Alfa Aesar
33.00	PHYSPROP

2-acetamidobenzoic acid C9H9NO3[2, 3, 64]



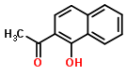
Compound Data

Melting point	**185.17 °C**	**458.32 K**			
CSID	6705	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	179.1727	**H bond donors**	2	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=C(Nc1ccccc1C(=O)O)C				
STD InChIKey	QSACCXVHEVWNMX-UHFFFAOYAX				

Melting Points

mp °C	source
184.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
186.00	Alfa Aesar
185.50	PHYSPROP

2-acetyl-1-naphthol C12H10O2[3, 64]



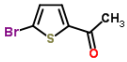
Compound Data

Melting point	**100.00 °C**	**373.15 K**			
CSID	62933	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	1	**ACD/LogP**	3.19
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	O=C(c2ccc1ccccc1c2O)C				
STD InChIKey	JBGJVMVWYWUVOW-UHFFFAOYAT				

Melting Points

mp °C	source
99.00	Alfa Aesar
101.00	PHYSPROP

2-acetyl-5-bromothiophene C6H5BrOS[3, 64]



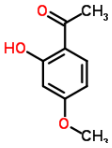
Compound Data

Melting point	**94.75 °C**	**367.90 K**			
CSID	71655	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	205.0723	**H bond donors**	0	**ACD/LogP**	2.25
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.62 g/cm^3
SMILES	O=C(c1sc(Br)cc1)C				
STD InChIKey	IGBZCOWXSCWSHO-UHFFFAOYAH				

Melting Points

mp °C	source
95.00	Alfa Aesar
94.50	PHYSPROP

2-acetyl-5-methoxy-phenol C9H10O3[3, 64]



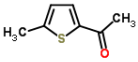
Compound Data

Melting point	**50.75 °C**	**323.90 K**			
CSID	10621	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	2.16
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	O=C(c1ccc(OC)cc1O)C				
STD InChIKey	UILPJVPSNHJFIK-UHFFFAOYAG				

Melting Points

mp °C	source
49.00	Alfa Aesar
52.50	PHYSPROP

2-acetyl-5-methylthiophene C7H8OS[3, 64]



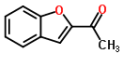
Compound Data

Melting point	**26.75 °C**	**299.90 K**			
CSID	75479	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	140.2028	**H bond donors**	0	**ACD/LogP**	1.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	O=C(c1sc(cc1)C)C				
STD InChIKey	YOSDTJYMDAEEAZ-UHFFFAOYAY				

Melting Points

mp °C	source
26.00	Alfa Aesar
27.50	PHYSPROP

2-acetylbenzo[b]furan C10H8O2[3, 64]



Compound Data

Melting point	**73.50 °C**	**346.65 K**			
CSID	14690	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.1693	**H bond donors**	0	**ACD/LogP**	2.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	O=C(c2oc1ccccc1c2)C				
STD InChIKey	YUTFQTAITWWGFH-UHFFFAOYAN				

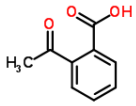
Melting Points

mp °C	source
71.00	Alfa Aesar
76.00	PHYSPROP

2-acetylbenzoic acid C9H8O3[2, 3, 64]

Compound Data

Melting point	**115.83 °C**	**388.98 K**



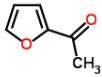
CSID	61749	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	164.158	**H bond donors**	1	**ACD/LogP**	0.81
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C(O)c1ccccc1C(=O)C				
STD InChIKey	QDAWXRKTSATEOP-UHFFFAOYAX				

Melting Points

mp °C	source
116.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
117.00	Alfa Aesar
114.50	PHYSPROP

2-acetylfuran C6H6O2[3, 61, 64]

Compound Data



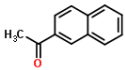
Melting point	**30.50 °C**	**303.65 K**			
CSID	13849	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	110.1106	**H bond donors**	0	**ACD/LogP**	0.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.06 g/cm^3
SMILES	O=C(c1occc1)C				
STD InChIKey	IEMMBWWQXVXBEU-UHFFFAOYAG				

Melting Points

mp °C	source
29.00	Alfa Aesar
29.50	Oxford University MSDS
33.00	PHYSPROP

2-acetylnaphthalene C12H10O[2, 3, 48, 64]

Compound Data



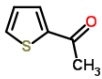
Melting point	**54.50 °C**	**327.65 K**			
CSID	6855	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2072	**H bond donors**	0	**ACD/LogP**	2.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.10 g/cm^3
SMILES	O=C(c2ccc1c(cccc1)c2)C				
STD InChIKey	XSAYZAUNJMRRIR-UHFFFAOYAQ				

Melting Points

mp °C	source
53.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
55.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
56.00	PHYSPROP

2-acetylthiophene C6H6OS[3, 64]

Compound Data

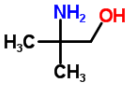


Melting point	**10.25 °C**	**283.40 K**			
CSID	6654	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	126.1762	**H bond donors**	0	**ACD/LogP**	1.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	O=C(c1sccc1)C				
STD InChIKey	WYJOVVXUZNRJQY-UHFFFAOYAB				

Melting Points

mp °C	source
10.00	Alfa Aesar
10.50	PHYSPROP

2-amino-2-methyl-1-propanol C4H11NO[3, 61, 64]



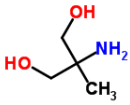
Compound Data

Melting point	**27.17 °C**	**300.32 K**			
CSID	13835861	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	89.1362	**H bond donors**	3	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.93 g/cm^3
SMILES	CC(C)(N)CO				
STD InChIKey	CBTVGIZVANVGBH-UHFFFAOYAK				

Melting Points

mp °C	source
26.00	Alfa Aesar
30.00	Oxford University MSDS
25.50	PHYSPROP

2-amino-2-methyl-1,3-propanediol C4H11NO2[61, 64]



Compound Data

Melting point	**110.50 °C**	**383.65 K**			
CSID	1477	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	105.1356	**H bond donors**	4	**ACD/LogP**	-1.17
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.13 g/cm^3
SMILES	OCC(N)(C)CO				
STD InChIKey	UXFQFBNBSPQBJW-UHFFFAOYAW				

Melting Points

mp °C	source
111.00	Oxford University MSDS
110.00	PHYSPROP

2-amino-3-methylpyridine C6H8N2[3, 64]

Compound Data

Melting point	**32.25 °C**	**305.40 K**			
CSID	14608	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	2	**ACD/LogP**	1.08
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	n1cccc(c1N)C				
STD InChIKey	RGDQRXPEZUNWHX-UHFFFAOYAS				

Melting Points

mp °C	source
31.00	Alfa Aesar
33.50	PHYSPROP

2-amino-3,6-dichlorobenzoic acid C7H5Cl2NO2[3, 64]

Compound Data

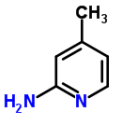
Melting point	**153.50 °C**	**426.65 K**			
CSID	525531	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	206.0261	**H bond donors**	3	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.61 g/cm^3
SMILES	Clc1ccc(Cl)c(C(=O)O)c1N				
STD InChIKey	MMIREQFMYZQWLU-UHFFFAOYAF				

Melting Points

mp °C	source
152.00	Alfa Aesar
155.00	PHYSPROP

2-amino-4-methylpyridine C6H8N2[3, 64]

Compound Data



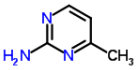
Melting point	**99.50 °C**	**372.65 K**			
CSID	1479	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	2	**ACD/LogP**	1.08
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	n1ccc(cc1N)C				
STD InChIKey	ORLGLBZRQYOWNA-UHFFFAOYAS				

Melting Points

mp °C	source
99.00	Alfa Aesar
100.00	PHYSPROP

2-amino-4-methylpyrimidine C5H7N3[3, 64]

Compound Data



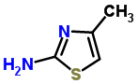
Melting point	**160.15 °C**	**433.30 K**			
CSID	7651	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	109.1292	**H bond donors**	2	**ACD/LogP**	0.24
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	n1c(ccnc1N)C				
STD InChIKey	GHCFWKFREBNSPC-UHFFFAOYAO				

Melting Points

mp °C	source
160.00	Alfa Aesar
160.30	PHYSPROP

2-amino-4-methylthiazole C4H6N2S[3, 64]

Compound Data



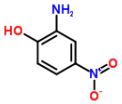
Melting point	**44.75 °C**	**317.90 K**			
CSID	66754	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.1688	**H bond donors**	2	**ACD/LogP**	1.77
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	Cc1csc(n1)N				
STD InChIKey	OUQMXTJYCAJLGO-UHFFFAOYAM				

Melting Points

mp °C	source
44.00	Alfa Aesar
45.50	PHYSPROP

2-amino-4-nitrophenol C6H6N2O3[2, 2, 3, 64]

Compound Data



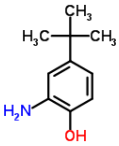
Melting point	**143.50 °C**	**416.65 K**			
CSID	2848685	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	154.1234	**H bond donors**	3	**ACD/LogP**	1.23
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.51 g/cm^3
SMILES	[O-][N+](=O)c1ccc(O)c(N)c1				
STD InChIKey	VLZVIIYRNMWPSN-UHFFFAOYAN				

Melting Points

mp °C	source
143.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
144.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
143.00	Alfa Aesar
144.00	PHYSPROP

2-amino-4-t-butylphenol C10H15NO[3, 64]

Compound Data



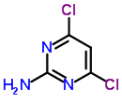
Melting point	**162.00 °C**	**435.15 K**			
CSID	64143	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	165.2322	**H bond donors**	3	**ACD/LogP**	2.13
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3
SMILES	Oc1ccc(cc1N)C(C)(C)C				
STD InChIKey	RPJUVNYXHUCRMG-UHFFFAOYAH				

Melting Points

mp °C	source
163.00	Alfa Aesar
161.00	PHYSPROP

2-amino-4,6-dichloropyrimidine C4H3Cl2N3[3, 64]

Compound Data



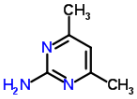
Melting point	**220.25 °C**	**493.40 K**			
CSID	58968	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	163.9927	**H bond donors**	2	**ACD/LogP**	0.98
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.61 g/cm^3
SMILES	Clc1nc(nc(Cl)c1)N				
STD InChIKey	JPZOAVGMSDSWSW-UHFFFAOYAI				

Melting Points

mp °C	source
220.00	Alfa Aesar
220.50	PHYSPROP

2-amino-4,6-dimethylpyrimidine C6H9N3[3, 64]

Compound Data



Melting point	**152.50 °C**	**425.65 K**			
CSID	12480	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	123.1558	**H bond donors**	2	**ACD/LogP**	0.70
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	n1c(cc(nc1N)C)C				
STD InChIKey	IDQNBVFPZMCDDN-UHFFFAOYAZ				

Melting Points

mp °C	source
153.00	Alfa Aesar
152.00	PHYSPROP

2-amino-5-chlorobenzonitrile C7H5ClN2[3, 64]

Compound Data

Melting point	**96.50 °C**	**369.65 K**			
CSID	72274	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	152.581	**H bond donors**	2	**ACD/LogP**	2.32
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	Clc1cc(C#N)c(N)cc1				
STD InChIKey	QYRDWARBHMCOAG-UHFFFAOYAW				

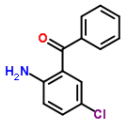
Melting Points

mp °C	source
96.00	Alfa Aesar
97.00	PHYSPROP

2-amino-5-chlorobenzophenone C13H10ClNO[3, 61, 64]

Compound Data

Melting point	**97.67 °C**	**370.82 K**			
CSID	12339	**H bond acceptors**	2	**Rule of 5 violations**	0



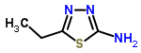
Molecular weight	231.6776	**H bond donors**	2	**ACD/LogP**	3.52
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	Clc2cc(C(=O)c1ccccc1)c(N)cc2				
STD InChIKey	ZUWXHHBROGLWNH-UHFFFAOYAQ				

Melting Points

mp °C	source
98.00	Alfa Aesar
96.00	Oxford University MSDS
99.00	PHYSPROP

2-amino-5-ethyl-1,3,4-thiadiazole C4H7N3S[3, 47]

Compound Data



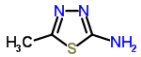
Melting point	**200.68 °C**	**473.82 K**			
CSID	24633	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	129.1835	**H bond donors**	2	**ACD/LogP**	0.37
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.28 g/cm^3
SMILES	n1nc(sc1CC)N				
STD InChIKey	QXTRPGAMVIONMK-UHFFFAOYAZ				

Melting Points

mp °C	source
200.00	Alfa Aesar
201.35	IUCr

2-amino-5-methyl-1,3,4-thiadiazole C3H5N3S[47, 64]

Compound Data



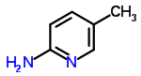
Melting point	**224.68 °C**	**497.82 K**			
CSID	60308	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	115.1569	**H bond donors**	2	**ACD/LogP**	-0.16
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.37 g/cm^3
SMILES	n1nc(sc1C)N				
STD InChIKey	HMPUHXCGUHDVBI-UHFFFAOYAV				

Melting Points

mp °C	source
224.85	IUCr
224.50	PHYSPROP

2-amino-5-methylpyridine C6H8N2[3, 64]

Compound Data



Melting point	**76.25 °C**	**349.40 K**			
CSID	14609	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	2	**ACD/LogP**	1.08
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	n1cc(ccc1N)C				
STD InChIKey	CMBSSVKZOPZBKW-UHFFFAOYAR				

Melting Points

mp °C	source
76.00	Alfa Aesar
76.50	PHYSPROP

2-amino-5-nitrobenzophenone C13H10N2O3[3, 64]

Compound Data

Melting point	**165.00 °C**	**438.15 K**

CSID	14916	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	242.2301	**H bond donors**	2	**ACD/LogP**	3.05
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.33 g/cm^3
SMILES	O=C(c1cc(ccc1N)[N+](=O)[O-])c2ccccc2				
STD InChIKey	PZPZDEIASIKHPY-UHFFFAOYAO				

Melting Points

mp °C	source
167.00	Alfa Aesar
163.00	PHYSPROP

2-amino-5-nitropyridine C5H5N3O2[3, 64]

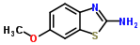
Compound Data

Melting point	**187.50 °C**	**460.65 K**			
CSID	70280	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	139.1121	**H bond donors**	2	**ACD/LogP**	1.18
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.44 g/cm^3
SMILES	c1cc(ncc1[N+](=O)[O-])N				
STD InChIKey	UGSBCCAHDVCHGI-UHFFFAOYAS				

Melting Points

mp °C	source
188.00	Alfa Aesar
187.00	PHYSPROP

2-amino-6-methoxybenzothiazole C8H8N2OS[3, 61, 64]



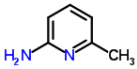
Compound Data

Melting point	**165.00 °C**	**438.15 K**			
CSID	14869	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2269	**H bond donors**	2	**ACD/LogP**	1.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	COc1ccc2c(c1)sc(n2)N				
STD InChIKey	KZHGPDSVHSDCMX-UHFFFAOYAT				

Melting Points

mp °C	source
163.00	Alfa Aesar
166.00	Oxford University MSDS
166.00	PHYSPROP

2-amino-6-methylpyridine C6H8N2[3, 64]



Compound Data

Melting point	**42.00 °C**	**315.15 K**			
CSID	14991	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	2	**ACD/LogP**	1.08
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	n1c(cccc1N)C				
STD InChIKey	QUXLCYFNVNNRBE-UHFFFAOYAI				

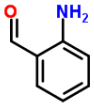
Melting Points

mp °C	source
43.00	Alfa Aesar
41.00	PHYSPROP

2-aminobenzaldehyde C7H7NO[2, 64]

Compound Data

Melting point	**38.50 °C**	**311.65 K**



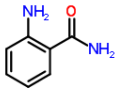
CSID	61553	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	121.1366	**H bond donors**	2	**ACD/LogP**	1.31
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=Cc1ccccc1N				
STD InChIKey	FXWFZIRWWNPPOV-UHFFFAOYAM				

Melting Points

mp °C	source
38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
39.00	PHYSPROP

2-aminobenzamide C7H8N2O[2, 2, 3]

Compound Data



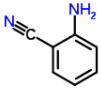
Melting point	**111.00 °C**	**384.15 K**			
CSID	10298355	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	136.1512	**H bond donors**	4	**ACD/LogP**	0.45
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C(N)c1ccccc1N				
STD InChIKey	PXBFMLJZNCDSMP-UHFFFAOYAZ				

Melting Points

mp °C	source
108.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
113.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
112.00	Alfa Aesar

2-aminobenzonitrile C7H6N2[2, 3, 64]

Compound Data



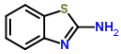
Melting point	**48.67 °C**	**321.82 K**			
CSID	65745	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1359	**H bond donors**	2	**ACD/LogP**	1.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	N#Cc1ccccc1N				
STD InChIKey	HLCPWBZNUKCSBN-UHFFFAOYAV				

Melting Points

mp °C	source
48.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
47.00	Alfa Aesar
51.00	PHYSPROP

2-aminobenzothiazole C7H6N2S[3, 64]

Compound Data



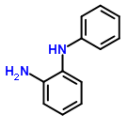
Melting point	**130.00 °C**	**403.15 K**			
CSID	8382	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.2009	**H bond donors**	2	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.38 g/cm^3
SMILES	n1c2ccccc2sc1N				
STD InChIKey	UHGULLIUJBCTEF-UHFFFAOYAA				

Melting Points

mp °C	source
128.00	Alfa Aesar
132.00	PHYSPROP

2-aminodiphenylamine C12H12N2[3, 64]

Compound Data



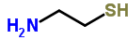
Melting point	**79.25 °C**	**352.40 K**			
CSID	61594	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	184.2371	**H bond donors**	3	**ACD/LogP**	2.02
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	c2c(Nc1ccccc1N)cccc2				
STD InChIKey	NFCPRRWCTNLGSN-UHFFFAOYAG				

Melting Points

mp °C	source
79.00	Alfa Aesar
79.50	PHYSPROP

2-aminoethanethiol C2H7NS[61, 64]

Compound Data



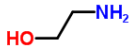
Melting point	**97.00 °C**	**370.15 K**			
CSID	5834	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	77.1487	**H bond donors**	2	**ACD/LogP**	0.03
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.97 g/cm^3
SMILES	SCCN				
STD InChIKey	UFULAYFCSOUIOV-UHFFFAOYAX				

Melting Points

mp °C	source
96.00	Oxford University MSDS
98.00	PHYSPROP

2-aminoethanol C2H7NO[3, 61, 64]

Compound Data



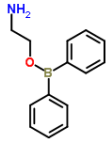
Melting point	**10.43 °C**	**283.58 K**			
CSID	13835336	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	61.0831	**H bond donors**	3	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.97 g/cm^3
SMILES	C(CO)N				
STD InChIKey	HZAXFHJVJLSVMW-UHFFFAOYAD				

Melting Points

mp °C	source
10.00	Alfa Aesar
11.00	Oxford University MSDS
10.30	PHYSPROP

2-aminoethyl diphenylborinate C14H16BNO[3, 64]

Compound Data



Melting point	**191.00 °C**	**464.15 K**			
CSID	1540	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	225.0939	**H bond donors**	2	**ACD/LogP**	3.48
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.04 g/cm^3
SMILES	O(B(c1ccccc1)c2ccccc2)CCN				
STD InChIKey	BLZVCIGGICSWIG-UHFFFAOYAJ				

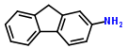
Melting Points

mp °C	source
189.00	Alfa Aesar
193.00	PHYSPROP

2-aminofluorene C13H11N[3, 64]

Compound Data

Melting point	**128.50 °C**	**401.65 K**	



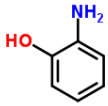
CSID	1484	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	181.2331	**H bond donors**	2	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.20 g/cm^3
SMILES	c1cccc3c1c2c(cc(N)cc2)C3				
STD InChIKey	CFRFHWQYWJMEJN-UHFFFAOYAE				

Melting Points

mp °C	source
128.00	Alfa Aesar
129.00	PHYSPROP

2-aminophenol C6H7NO[2, 3, 32, 64]

Compound Data



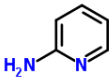
Melting point	**174.75 °C**	**447.90 K**			
CSID	5596	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	3	**ACD/LogP**	0.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	c1ccc(c(c1)N)O				
STD InChIKey	CDAWCLOXVUBKRW-UHFFFAOYAP				

Melting Points

mp °C	source
176.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
175.00	Alfa Aesar
174.00	DrugBank
174.00	PHYSPROP

2-aminopyridine C5H6N2[3, 64]

Compound Data



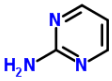
Melting point	**57.75 °C**	**330.90 K**			
CSID	10008	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.1145	**H bond donors**	2	**ACD/LogP**	0.53
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c1ccnc(c1)N				
STD InChIKey	ICSNLGPSRYBMBD-UHFFFAOYAM				

Melting Points

mp °C	source
58.00	Alfa Aesar
57.50	PHYSPROP

2-aminopyrimidine C4H5N3[3, 64]

Compound Data



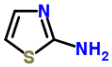
Melting point	**126.25 °C**	**399.40 K**			
CSID	7690	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	95.1026	**H bond donors**	2	**ACD/LogP**	-0.22
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.22 g/cm^3
SMILES	c1cnc(nc1)N				
STD InChIKey	LJXQPZWIHJMPQQ-UHFFFAOYAJ				

Melting Points

mp °C	source
125.00	Alfa Aesar
127.50	PHYSPROP

2-aminothiazole C3H4N2S[3, 64]

Compound Data



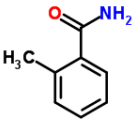
Melting point	**91.50 °C**	**364.65 K**			
CSID	2070	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1423	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.35 g/cm^3
SMILES	c1csc(n1)N				
STD InChIKey	RAIPHJJURHTUIC-UHFFFAOYAZ				

Melting Points

mp °C	source
90.00	Alfa Aesar
93.00	PHYSPROP

2-aminotoluene C8H9NO[2, 64]

Compound Data



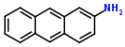
Melting point	**144.50 °C**	**417.65 K**			
CSID	10254	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	2	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	O=C(c1ccccc1C)N				
STD InChIKey	XXUNIGZDNWWYED-UHFFFAOYAM				

Melting Points

mp °C	source
142.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
147.00	PHYSPROP

2-anthracenamine C14H11N[3, 61, 64]

Compound Data



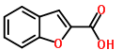
Melting point	**236.93 °C**	**510.08 K**			
CSID	11443	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	193.2438	**H bond donors**	2	**ACD/LogP**	3.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	c3ccc2cc1ccc(N)cc1cc2c3				
STD InChIKey	YCSBALJAGZKWFF-UHFFFAOYAR				

Melting Points

mp °C	source
237.00	Alfa Aesar
235.00	Oxford University MSDS
238.80	PHYSPROP

2-benzofurancarboxylic acid C9H6O3[3, 64]

Compound Data



Melting point	**193.25 °C**	**466.40 K**			
CSID	10778469	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	162.1421	**H bond donors**	1	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	c1ccc2c(c1)cc(o2)C(=O)O				
STD InChIKey	OFFSPAZVIVZPHU-UHFFFAOYAU				

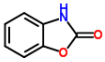
Melting Points

mp °C	source
194.00	Alfa Aesar
192.50	PHYSPROP

2-benzoxazolinone C7H5NO2[3, 64]

Compound Data

Melting point	**139.00 °C**	**412.15 K**

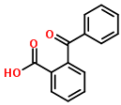


CSID	5820	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	135.1201	**H bond donors**	1	**ACD/LogP**	1.16
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.32 g/cm^3
SMILES	O=C2Oc1ccccc1N2				
STD InChIKey	ASSKVPFEZFQQNQ-UHFFFAOYAD				

Melting Points

mp °C	source
140.00	Alfa Aesar
138.00	PHYSPROP

2-benzoylbenzoic acid C14H10O3[3, 64]



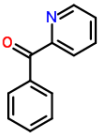
Compound Data

Melting point	**128.00 °C**	**401.15 K**			
CSID	6554	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.2274	**H bond donors**	1	**ACD/LogP**	2.31
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.26 g/cm^3
SMILES	O=C(O)c2ccccc2C(=O)c1ccccc1				
STD InChIKey	FGTYTUFKXYPTML-UHFFFAOYAN				

Melting Points

mp °C	source
129.00	Alfa Aesar
127.00	PHYSPROP

2-benzoylpyridine C12H9NO[3, 64]



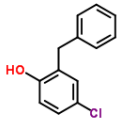
Compound Data

Melting point	**42.50 °C**	**315.65 K**			
CSID	6771	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	183.206	**H bond donors**	0	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(c1ccccc1)c2ncccc2				
STD InChIKey	GCSHUYKULREZSJ-UHFFFAOYAK				

Melting Points

mp °C	source
43.00	Alfa Aesar
42.00	PHYSPROP

2-benzyl-4-chlorophenol C13H11ClO[3, 64]



Compound Data

Melting point	**48.25 °C**	**321.40 K**			
CSID	8118	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	218.6788	**H bond donors**	1	**ACD/LogP**	4.42
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	Clc1cc(c(O)cc1)Cc2ccccc2				
STD InChIKey	NCKMMSIFQUPKCK-UHFFFAOYAC				

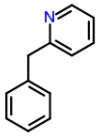
Melting Points

mp °C	source
48.00	Alfa Aesar
48.50	PHYSPROP

2-benzylpyridine C12H11N[3, 64]

Compound Data

Melting point	**11.25 °C**	**284.40 K**			
CSID	7300	**H bond acceptors**	1	**Rule of 5 violations**	0



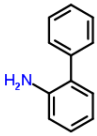
Molecular weight	169.2224	**H bond donors**	0	**ACD/LogP**	2.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	n1ccccc1Cc2ccccc2				
STD InChIKey	PCFUWBOSXMKGIP-UHFFFAOYAU				

Melting Points

mp °C	source
10.00	Alfa Aesar
12.50	PHYSPROP

2-biphenylamine C12H11N[3, 7, 61, 64]

Compound Data



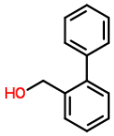
Melting point	**50.38 °C**	**323.52 K**			
CSID	6748	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	169.2224	**H bond donors**	2	**ACD/LogP**	2.68
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.08 g/cm^3
SMILES	c2c(c1ccccc1N)cccc2				
STD InChIKey	TWBPWBPGNQWFSJ-UHFFFAOYAD				

Melting Points

mp °C	source
50.00	Alfa Aesar
49.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
51.50	Oxford University MSDS
51.00	PHYSPROP

2-biphenylmethanol C13H12O[3, 7]

Compound Data



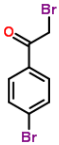
Melting point	**49.50 °C**	**322.65 K**			
CSID	68709	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.2338	**H bond donors**	1	**ACD/LogP**	2.79
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.09 g/cm^3
SMILES	OCc2ccccc2c1ccccc1				
STD InChIKey	VKTQADPEPIVMHK-UHFFFAOYAA				

Melting Points

mp °C	source
49.00	Alfa Aesar
50.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

2-bromo-1-(4-bromophenyl)ethanone C8H6Br2O[3, 61, 64]

Compound Data

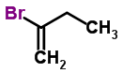


Melting point	**110.00 °C**	**383.15 K**			
CSID	7174	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	277.9406	**H bond donors**	0	**ACD/LogP**	2.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.85 g/cm^3
SMILES	O=C(c1ccc(Br)cc1)CBr				
STD InChIKey	FKJSFKCZZIXQIP-UHFFFAOYAM				

Melting Points

mp °C	source
110.00	Alfa Aesar
109.00	Oxford University MSDS
111.00	PHYSPROP

2-bromo-1-butene C4H7Br[31, 64]



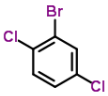
Compound Data

Melting point	**-133.20 °C**	**139.95 K**			
CSID	81237	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	135.0024	**H bond donors**	0	**ACD/LogP**	2.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.31 g/cm^3
SMILES	Br/C(=C)CC				
STD InChIKey	HQMXRIGBXOFKIU-UHFFFAOYAJ				

Melting Points

mp °C	source
-133.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-133.40	PHYSPROP

2-bromo-1,4-dichlorobenzene C6H3BrCl2[3, 64]



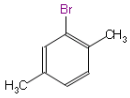
Compound Data

Melting point	**34.50 °C**	**307.65 K**			
CSID	14309	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	225.898	**H bond donors**	0	**ACD/LogP**	3.97
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.74 g/cm^3
SMILES	Clc1cc(Br)c(Cl)cc1				
STD InChIKey	OVXVQBCRONSPDC-UHFFFAOYAH				

Melting Points

mp °C	source
34.00	Alfa Aesar
35.00	PHYSPROP

2-bromo-1,4-dimethylbenzene C8H9Br[2, 3, 64]



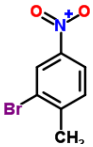
Compound Data

Melting point	**9.67 °C**	**282.82 K**			
CSID	21171515	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	185.0611	**H bond donors**	0	**ACD/LogP**	3.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.34 g/cm^3
SMILES	Cc1cc(Br)c(C)cc1				
STD InChIKey	QXISTPDUYKNPLU-UHFFFAOYAG				

Melting Points

mp °C	source
10.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
10.00	Alfa Aesar
9.00	PHYSPROP

2-bromo-4-nitrotoluene C7H6BrNO2[2, 3, 64]



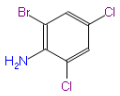
Compound Data

Melting point	**76.67 °C**	**349.82 K**			
CSID	74171	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	216.032	**H bond donors**	0	**ACD/LogP**	2.98
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.61 g/cm^3
SMILES	Brc1cc([N+]([O-])=O)ccc1C				
STD InChIKey	XFZFJQHXWJIBQV-UHFFFAOYAP				

Melting Points

mp °C	source
76.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
76.00	Alfa Aesar
78.00	PHYSPROP

2-bromo-4,6-dichloroaniline C6H4BrCl2N[3, 64]



Compound Data

Melting point	**81.75 °C**	**354.90 K**			
CSID	21168862	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	240.9127	**H bond donors**	2	**ACD/LogP**	3.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.83 g/cm^3
SMILES	Clc1cc(Cl)cc(Br)c1N				
STD InChIKey	DTPADCOGQUOGHT-UHFFFAOYAD				

Melting Points

mp °C	source
80.00	Alfa Aesar
83.50	PHYSPROP

2-bromo-4,6-dinitroaniline C6H4BrN3O4[3, 64]

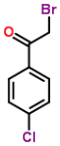
Compound Data

Melting point	**152.75 °C**	**425.90 K**			
CSID	14979	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	262.0177	**H bond donors**	2	**ACD/LogP**	3.09
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.99 g/cm^3
SMILES	Brc1cc(cc([N+]([O-])=O)c1N)[N+]([O-])=O				
STD InChIKey	KWMDHCLJYMVBNS-UHFFFAOYAM				

Melting Points

mp °C	source
152.00	Alfa Aesar
153.50	PHYSPROP

2-bromo-4'-chloroacetophenone C8H6BrClO[3, 64]



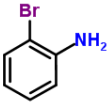
Compound Data

Melting point	**96.25 °C**	**369.40 K**			
CSID	61599	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	233.4896	**H bond donors**	0	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=C(c1ccc(Cl)cc1)CBr				
STD InChIKey	FLAYZKKEOIAALB-UHFFFAOYAA				

Melting Points

mp °C	source
96.00	Alfa Aesar
96.50	PHYSPROP

2-bromoaniline C6H6BrN[2, 3, 64]



Compound Data

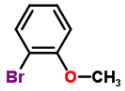
Melting point	**30.33 °C**	**303.48 K**			
CSID	21111816	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	172.0225	**H bond donors**	2	**ACD/LogP**	2.19
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.59 g/cm^3
SMILES	Nc1ccccc1Br				
STD InChIKey	AOPBDRUWRLBSDB-UHFFFAOYAG				

Melting Points

mp °C	source
30.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
29.00	Alfa Aesar
32.00	PHYSPROP

2-bromoanisole C7H7BrO[2, 3, 64]

Compound Data



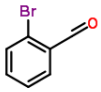
Melting point	**2.50 °C**	**275.65 K**			
CSID	13881329	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	187.0339	**H bond donors**	0	**ACD/LogP**	2.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.44 g/cm^3
SMILES	COc1ccccc1Br				
STD InChIKey	HTDQSWDEWGSAMN-UHFFFAOYAQ				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
3.00	Alfa Aesar
2.50	PHYSPROP

2-bromobenzaldehyde C7H5BrO[2, 3, 64]

Compound Data



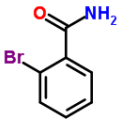
Melting point	**21.17 °C**	**294.32 K**			
CSID	21111817	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	185.018	**H bond donors**	0	**ACD/LogP**	2.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.58 g/cm^3
SMILES	O=Cc1ccccc1Br				
STD InChIKey	NDOPHXWIAZIXPR-UHFFFAOYAE				

Melting Points

mp °C	source
22.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
20.00	Alfa Aesar
21.50	PHYSPROP

2-bromobenzamide C7H6BrNO[2, 3, 64]

Compound Data



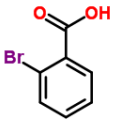
Melting point	**160.50 °C**	**433.65 K**			
CSID	70021	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.0326	**H bond donors**	2	**ACD/LogP**	0.73
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.61 g/cm^3
SMILES	O=C(c1ccccc1Br)N				
STD InChIKey	NHNAEZDWNCRWRW-UHFFFAOYAZ				

Melting Points

mp °C	source
160.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
161.00	Alfa Aesar
160.50	PHYSPROP

2-bromobenzoic acid C7H5BrO2[2, 3, 64, 70]

Compound Data

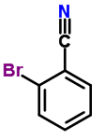


Melting point	**148.25 °C**	**421.40 K**			
CSID	6674	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	201.0174	**H bond donors**	1	**ACD/LogP**	2.15
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.70 g/cm^3
SMILES	O=C(O)c1ccccc1Br				
STD InChIKey	XRXMNWGCKISMOH-UHFFFAOYAG				

Melting Points

mp °C	source
149.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
148.00	Alfa Aesar
150.00	PHYSPROP
146.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

2-bromobenzonitrile C_7H_4BrN[2, 3, 64]



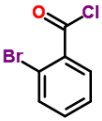
Compound Data

Melting point	**55.17 °C**	**328.32 K**			
CSID	15440	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.0174	**H bond donors**	0	**ACD/LogP**	2.23
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.60 g/cm^3
SMILES	N#Cc1ccccc1Br				
STD InChIKey	AFMPMSCZPVNPEM-UHFFFAOYAE				

Melting Points

mp °C	source
55.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
55.50	PHYSPROP

2-bromobenzoyl chloride C_7H_4BrClO[3, 64]



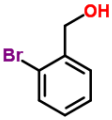
Compound Data

Melting point	**10.50 °C**	**283.65 K**			
CSID	22012	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	219.4631	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.66 g/cm^3
SMILES	O=C(Cl)c1ccccc1Br				
STD InChIKey	NZCKTGCKFJDGFD-UHFFFAOYAT				

Melting Points

mp °C	source
10.00	Alfa Aesar
11.00	PHYSPROP

2-bromobenzyl alcohol C_7H_7BrO[2, 3]



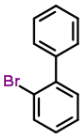
Compound Data

Melting point	**80.50 °C**	**353.65 K**			
CSID	65682	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	187.0339	**H bond donors**	1	**ACD/LogP**	1.81
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.56 g/cm^3
SMILES	Brc1ccccc1CO				
STD InChIKey	IOWGHQGLUMEZKG-UHFFFAOYAE				

Melting Points

mp °C	source
81.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
80.00	Alfa Aesar

2-bromobiphenyl $C_{12}H_9Br$[2, 3, 64]



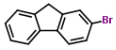
Compound Data

Melting point	**1.50 °C**	**274.65 K**			
CSID	15494	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	233.1039	**H bond donors**	0	**ACD/LogP**	4.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	Brc2ccccc2c1ccccc1				
STD InChIKey	KTADSLDAUJLZGL-UHFFFAOYAT				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
1.00	Alfa Aesar
1.50	PHYSPROP

2-bromofluorene $C_{13}H_9Br$[3, 64]



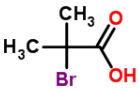
Compound Data

Melting point	**112.75 °C**	**385.90 K**			
CSID	13697	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	245.1146	**H bond donors**	0	**ACD/LogP**	4.93
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	Brc3ccc2c1ccccc1Cc2c3				
STD InChIKey	FXSCJZNMWILAJO-UHFFFAOYAS				

Melting Points

mp °C	source
112.00	Alfa Aesar
113.50	PHYSPROP

2-bromoisobutyric acid $C_4H_7BrO_2$[3, 64]



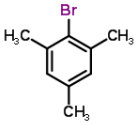
Compound Data

Melting point	**46.25 °C**	**319.40 K**			
CSID	10790335	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	167.0012	**H bond donors**	1	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.63 g/cm^3
SMILES	BrC(C)(C)C(O)=O				
STD InChIKey	XXSPGBOGLXKMDU-UHFFFAOYAO				

Melting Points

mp °C	source
44.00	Alfa Aesar
48.50	PHYSPROP

2-bromomesitylene $C_9H_{11}Br$[2, 3, 64]



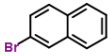
Compound Data

Melting point	**1.00 °C**	**274.15 K**			
CSID	21112244	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	199.0876	**H bond donors**	0	**ACD/LogP**	4.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	Cc1cc(C)c(Br)c(C)c1				
STD InChIKey	RRTLQRYOJOSPEA-UHFFFAOYAY				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
2.00	Alfa Aesar
-1.00	PHYSPROP

2-bromonaphthalene $C_{10}H_7Br$[2, 3, 64]



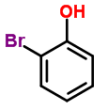
Compound Data

Melting point	**56.00 °C**	**329.15 K**			
CSID	10894	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	207.0666	**H bond donors**	0	**ACD/LogP**	4.22
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.48 g/cm^3
SMILES	Brc2ccc1c(cccc1)c2				
STD InChIKey	APSMUYYLXZULMS-UHFFFAOYAY				

Melting Points

mp °C	source
54.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
59.00	PHYSPROP

2-bromophenol C6H5BrO[2, 3, 32, 64]



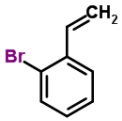
Compound Data

Melting point	**5.30 °C**	**278.45 K**			
CSID	6974	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	173.0073	**H bond donors**	1	**ACD/LogP**	2.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.66 g/cm^3
SMILES	Oc1ccccc1Br				
STD InChIKey	VADKRMSMGWJZCF-UHFFFAOYAR				

Melting Points

mp °C	source
5.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
5.00	Alfa Aesar
5.60	DrugBank
5.60	PHYSPROP

2-bromostyrene C8H7Br[3, 64]



Compound Data

Melting point	**-52.75 °C**	**220.40 K**			
CSID	15432	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	183.0452	**H bond donors**	0	**ACD/LogP**	3.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	C=Cc1ccccc1Br				
STD InChIKey	SSZOCHFYWWVSAI-UHFFFAOYAV				

Melting Points

mp °C	source
-53.00	Alfa Aesar
-52.50	PHYSPROP

2-bromotoluene C7H7Br[3, 31, 64]

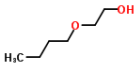
Compound Data

Melting point	**-27.60 °C**	**245.55 K**			
CSID	13875320	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	171.0345	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	Cc1ccccc1Br				
STD InChIKey	QSSXJPIWXQTSIX-UHFFFAOYAF				

Melting Points

mp °C	source
-27.00	Alfa Aesar
-28.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-27.80	PHYSPROP

2-butoxyethanol C6H14O2[3, 61, 64]



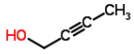
Compound Data

Melting point	**-76.27 °C**	**196.88 K**			
CSID	13836399	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1742	**H bond donors**	1	**ACD/LogP**	0.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.90 g/cm^3
SMILES	CCCCOCCO				
STD InChIKey	POAOYUHQDCAZBD-UHFFFAOYAB				

Melting Points

mp °C	source
-79.00	Alfa Aesar
-75.00	Oxford University MSDS
-74.80	PHYSPROP

2-butyn-1-ol C4H6O[3, 61, 64]



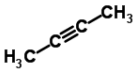
Compound Data

Melting point	**-2.13 °C**	**271.02 K**			
CSID	12450	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	70.0898	**H bond donors**	1	**ACD/LogP**	0.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.93 g/cm^3
SMILES	C(#CCO)C				
STD InChIKey	NEEDEQSZOUAJMU-UHFFFAOYAV				

Melting Points

mp °C	source
-2.00	Alfa Aesar
-2.20	Oxford University MSDS
-2.20	PHYSPROP

2-butyne C4H6[2, 3, 64]



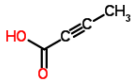
Compound Data

Melting point	**-32.10 °C**	**241.05 K**			
CSID	9990	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	54.0904	**H bond donors**	0	**ACD/LogP**	1.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.69 g/cm^3
SMILES	C(#CC)C				
STD InChIKey	XNMQEEKYCVKGBD-UHFFFAOYAO				

Melting Points

mp °C	source
-32.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-32.00	Alfa Aesar
-32.30	PHYSPROP

2-butynoic acid C4H4O2[3, 64]



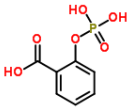
Compound Data

Melting point	**77.50 °C**	**350.65 K**			
CSID	61810	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	84.0734	**H bond donors**	1	**ACD/LogP**	0.85
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	O=C(C#CC)O				
STD InChIKey	LUEHNHVFDCZTGL-UHFFFAOYAN				

Melting Points

mp °C	source
77.00	Alfa Aesar
78.00	PHYSPROP

2-carboxyphenyl phosphate C7H7O6P[3, 9, 48, 64]



Compound Data

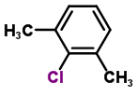
Melting point	**167.25 °C**	**440.40 K**			
CSID	3300	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	218.1006	**H bond donors**	3	**ACD/LogP**	-0.32
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.70 g/cm^3
SMILES	O=P(Oc1ccccc1C(=O)O)(O)O				
STD InChIKey	FFKUDWZICMJVPA-UHFFFAOYAO				

Melting Points

mp °C	source
164.00	Alfa Aesar
168.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...

168.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
169.00	PHYSPROP

2-chloro-1,3-dimethylbenzene C8H9Cl[3, 64]



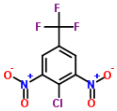
Compound Data

Melting point	**-35.50 °C**	**237.65 K**			
CSID	13875381	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	140.6101	**H bond donors**	0	**ACD/LogP**	3.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	Cc1cccc(C)c1Cl				
STD InChIKey	VDXLAYAQGYCQEO-UHFFFAOYAL				

Melting Points

mp °C	source
-36.00	Alfa Aesar
-35.00	PHYSPROP

2-chloro-1,3-dinitro-5-(trifluoromethyl)benzene C7H2ClF3N2O4[3, 61, 64]



Compound Data

Melting point	**56.67 °C**	**329.82 K**			
CSID	9426	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	270.55	**H bond donors**	0	**ACD/LogP**	2.64
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.71 g/cm^3
SMILES	O=[N+]([O-])c1cc(cc([N+]([O-])=O)c1Cl)C(F)(F)F				
STD InChIKey	HFHAVERNVFNSHL-UHFFFAOYAU				

Melting Points

mp °C	source
56.00	Alfa Aesar
57.00	Oxford University MSDS
57.00	PHYSPROP

2-chloro-1,3-dinitrobenzene C6H3ClN2O4[3, 64]

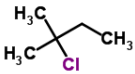
Compound Data

Melting point	**87.00 °C**	**360.15 K**			
CSID	21242790	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	202.552	**H bond donors**	0	**ACD/LogP**	1.79
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.62 g/cm^3
SMILES	O=[N+]([O-])c1cccc([N+]([O-])=O)c1Cl				
STD InChIKey	BPPMIQPXQVIZNJ-UHFFFAOYAA				

Melting Points

mp °C	source
86.00	Alfa Aesar
88.00	PHYSPROP

2-chloro-2-methylbutane C5H11Cl[3, 31, 61, 64]



Compound Data

Melting point	**-73.38 °C**	**199.77 K**			
CSID	55090	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.5938	**H bond donors**	0	**ACD/LogP**	2.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	ClC(C)(C)CC				
STD InChIKey	CRNIHJHMEQZAAS-UHFFFAOYAL				

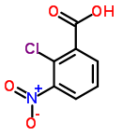
Melting Points

mp °C	source
-73.00	Alfa Aesar

-74.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-73.00	Oxford University MSDS
-73.50	PHYSPROP

2-chloro-3-nitrobenzoic acid C7H4ClNO4[2, 3, 64]

Compound Data



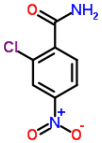
Melting point	**182.83 °C**	**455.98 K**			
CSID	18716	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	1	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=[N+]([O-])c1cccc(C(=O)O)c1Cl				
STD InChIKey	JRQDVRIQJJPHEQ-UHFFFAOYAE				

Melting Points

mp °C	source
181.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
184.00	Alfa Aesar
183.50	PHYSPROP

2-chloro-4-nitrobenzamide C7H5ClN2O3[3, 64]

Compound Data



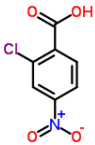
Melting point	**171.00 °C**	**444.15 K**			
CSID	1991	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	200.5792	**H bond donors**	2	**ACD/LogP**	1.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.52 g/cm^3
SMILES	O=C(c1ccc(cc1Cl)[N+]([O-])=O)N				
STD InChIKey	GFGSZUNNBQXGMK-UHFFFAOYAX				

Melting Points

mp °C	source
170.00	Alfa Aesar
172.00	PHYSPROP

2-chloro-4-nitrobenzoic acid C7H4ClNO4[2, 3, 64]

Compound Data



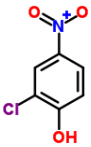
Melting point	**140.33 °C**	**413.48 K**			
CSID	7168	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	1	**ACD/LogP**	2.13
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=C(O)c1ccc(cc1Cl)[N+]([O-])=O				
STD InChIKey	QAYNSPOKTRVZRC-UHFFFAOYAQ				

Melting Points

mp °C	source
139.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
142.00	Alfa Aesar
140.00	PHYSPROP

2-chloro-4-nitrophenol C6H4ClNO3[2, 3]

Compound Data



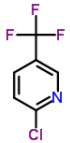
Melting point	**108.00 °C**	**381.15 K**			
CSID	11577	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	173.5539	**H bond donors**	1	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.55 g/cm^3
SMILES	Clc1cc([N+]([O-])=O)ccc1O				
STD InChIKey	BOFRXDMCQRTGII-UHFFFAOYAM				

Melting Points

mp °C	source
106.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
110.00	Alfa Aesar

2-chloro-5-(trifluoromethyl)pyridine C6H3ClF3N[3, 64]

Compound Data



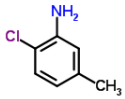
Melting point	**32.00 °C**	**305.15 K**			
CSID	83365	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	181.5429	**H bond donors**	0	**ACD/LogP**	2.31
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	c1cc(ncc1C(F)(F)F)Cl				
STD InChIKey	JFZJMSDDOOAOIV-UHFFFAOYAY				

Melting Points

mp °C	source
31.00	Alfa Aesar
33.00	PHYSPROP

2-chloro-5-methylaniline C7H8ClN[2, 3, 64]

Compound Data



Melting point	**30.83 °C**	**303.98 K**			
CSID	60136	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	141.5981	**H bond donors**	2	**ACD/LogP**	2.37
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Clc1ccc(cc1N)C				
STD InChIKey	HPSCXFOQUFPEPE-UHFFFAOYAA				

Melting Points

mp °C	source
31.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar
29.50	PHYSPROP

2-chloro-5-nitroaniline C6H5ClN2O2[2, 3, 64]

Compound Data

Melting point	**119.33 °C**	**392.48 K**			
CSID	21272	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.5691	**H bond donors**	2	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.49 g/cm^3
SMILES	Clc1ccc([N+]([O-])=O)cc1N				
STD InChIKey	KWIXNFOTNVKIGM-UHFFFAOYAZ				

Melting Points

mp °C	source
118.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
119.00	Alfa Aesar
121.00	PHYSPROP

2-chloro-5-nitrobenzoic acid C7H4ClNO4[2, 3, 35, 64]

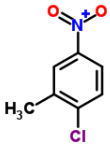
Compound Data

Melting point	**166.50 °C**	**439.65 K**			
CSID	16359	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	1	**ACD/LogP**	2.02
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=C(O)c1cc(ccc1Cl)[N+]([O-])=O				
STD InChIKey	QUEKGYQTRJVEQC-UHFFFAOYAV				

Melting Points

mp °C	source
166.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
167.00	Alfa Aesar
166.50	EPISuite-ChemSpider
166.50	PHYSPROP

2-chloro-5-nitrotoluene C7H6ClNO2[3, 64]



Compound Data

Melting point	**42.75 °C**	**315.90 K**			
CSID	75176	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	0	**ACD/LogP**	3.06
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	Clc1ccc([N+]([O-])=O)cc1C				
STD InChIKey	BGDCQZFFNFXYQC-UHFFFAOYAN				

Melting Points

mp °C	source
43.00	Alfa Aesar
42.50	PHYSPROP

2-chloro-6-fluorobenzoic acid C7H4ClFO2[3, 64]

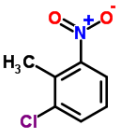
Compound Data

Melting point	**159.00 °C**	**432.15 K**			
CSID	61264	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	174.5569	**H bond donors**	1	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.48 g/cm^3
SMILES	O=C(O)c1c(F)cccc1Cl				
STD InChIKey	XNTIGDVFBDJLTQ-UHFFFAOYAU				

Melting Points

mp °C	source
158.00	Alfa Aesar
160.00	PHYSPROP

2-chloro-6-nitrotoluene C7H6ClNO2[2, 3, 64]



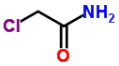
Compound Data

Melting point	**36.60 °C**	**309.75 K**			
CSID	6484	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	0	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	Clc1cccc([N+]([O-])=O)c1C				
STD InChIKey	XCSNRORTQRKCHB-UHFFFAOYAH				

Melting Points

mp °C	source
36.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
36.00	Alfa Aesar
37.80	PHYSPROP

2-chloroacetamide C2H4ClNO[3, 64]



Compound Data

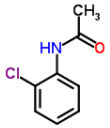
Melting point	**119.50 °C**	**392.65 K**			
CSID	6332	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	93.5123	**H bond donors**	2	**ACD/LogP**	-0.85
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	ClCC(=O)N				
STD InChIKey	VXIVSQZSERGHQP-UHFFFAOYAM				

Melting Points

mp °C	source
118.00	Alfa Aesar
121.00	PHYSPROP

2-chloroacetanilide C8H8ClNO[3, 64]

Compound Data



Melting point	**88.00 °C**	**361.15 K**			
CSID	10322	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	169.6082	**H bond donors**	1	**ACD/LogP**	1.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	Clc1ccccc1NC(=O)C				
STD InChIKey	KNVQTRVKSOEHPU-UHFFFAOYAW				

Melting Points

mp °C	source
87.00	Alfa Aesar
89.00	PHYSPROP

2-chloroacrylic acid C3H3ClO2[3, 64]

Compound Data

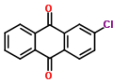
Melting point	**65.50 °C**	**338.65 K**			
CSID	11242	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	106.5077	**H bond donors**	1	**ACD/LogP**	0.43
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	Cl/C(=C)C(=O)O				
STD InChIKey	SZTBMYHIYNGYIA-UHFFFAOYAK				

Melting Points

mp °C	source
65.00	Alfa Aesar
66.00	PHYSPROP

2-chloroanthraquinone C14H7ClO2[3, 64]

Compound Data



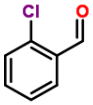
Melting point	**210.00 °C**	**483.15 K**			
CSID	8235	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	242.6572	**H bond donors**	0	**ACD/LogP**	4.11
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	Clc3ccc2C(=O)c1c(cccc1)C(=O)c2c3				
STD InChIKey	FPKCTSIVDAWGFA-UHFFFAOYAD				

Melting Points

mp °C	source
209.00	Alfa Aesar
211.00	PHYSPROP

2-chlorobenzaldehyde C7H5ClO[2, 3, 61, 64]

Compound Data



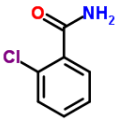
Melting point	**10.60 °C**	**283.75 K**			
CSID	21106014	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	140.567	**H bond donors**	0	**ACD/LogP**	2.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	O=Cc1ccccc1Cl				
STD InChIKey	FPYUJUBAXZAQNL-UHFFFAOYAV				

Melting Points

mp °C	source

11.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
10.00	Alfa Aesar
9.00	Oxford University MSDS
12.40	PHYSPROP

2-chlorobenzamide C7H6ClNO[2, 3, 64]



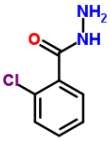
Compound Data

Melting point	**142.67 °C**	**415.82 K**			
CSID	62328	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	155.5816	**H bond donors**	2	**ACD/LogP**	0.93
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1ccccc1Cl)N				
STD InChIKey	RBGDLYUEXLWQBZ-UHFFFAOYAX				

Melting Points

mp °C	source
143.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
142.00	Alfa Aesar
143.00	PHYSPROP

2-chlorobenzhydrazide C7H7ClN2O[3, 64]



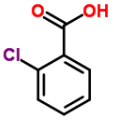
Compound Data

Melting point	**118.50 °C**	**391.65 K**			
CSID	72174	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	170.5963	**H bond donors**	3	**ACD/LogP**	0.14
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=C(c1ccccc1Cl)NN				
STD InChIKey	KPPNLSKVTKSSTG-UHFFFAOYAQ				

Melting Points

mp °C	source
118.00	Alfa Aesar
119.00	PHYSPROP

2-chlorobenzoic acid C7H5ClO2[2, 3, 61, 64]



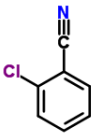
Compound Data

Melting point	**140.30 °C**	**413.45 K**			
CSID	8071	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.5664	**H bond donors**	1	**ACD/LogP**	2.04
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	O=C(O)c1ccccc1Cl				
STD InChIKey	IKCLCGXPQILATA-UHFFFAOYAI				

Melting Points

mp °C	source
139.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
140.00	Alfa Aesar
142.00	Oxford University MSDS
140.20	PHYSPROP

2-chlorobenzonitrile C7H4ClN[2, 3, 64]



Compound Data

Melting point	**45.43 °C**	**318.58 K**			
CSID	12818	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	137.5664	**H bond donors**	0	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3
SMILES	N#Cc1ccccc1Cl				

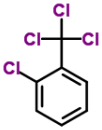
STD InChIKey	NHWQMJMIYICNBP-UHFFFAOYAP

Melting Points

mp °C	source
45.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
45.00	Alfa Aesar
46.30	PHYSPROP

2-chlorobenzotrichloride C7H4Cl4[3, 31, 64]

Compound Data



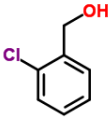
Melting point	**29.47 °C**	**302.62 K**			
CSID	15636	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	229.9187	**H bond donors**	0	**ACD/LogP**	3.94
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.50 g/cm^3
SMILES	ClC(Cl)(Cl)c1ccccc1Cl				
STD InChIKey	MFHPYLFZSCSNST-UHFFFAOYAH				

Melting Points

mp °C	source
30.00	Alfa Aesar
29.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
29.40	PHYSPROP

2-chlorobenzyl alcohol C7H7ClO[2, 3, 64]

Compound Data



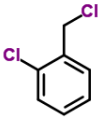
Melting point	**71.00 °C**	**344.15 K**			
CSID	26799	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	142.5829	**H bond donors**	1	**ACD/LogP**	1.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	Clc1ccccc1CO				
STD InChIKey	MBYQPPXEXWRMQC-UHFFFAOYAN				

Melting Points

mp °C	source
70.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
70.00	Alfa Aesar
73.00	PHYSPROP

2-chlorobenzyl chloride C7H6Cl2[3, 64]

Compound Data



Melting point	**-15.00 °C**	**258.15 K**			
CSID	11412	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	161.0285	**H bond donors**	0	**ACD/LogP**	3.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	ClCc1ccccc1Cl				
STD InChIKey	BASMANVIUSSIIM-UHFFFAOYAQ				

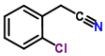
Melting Points

mp °C	source
-13.00	Alfa Aesar
-17.00	PHYSPROP

2-chlorobenzyl cyanide C8H6ClN[2, 3, 64]

Compound Data

Melting point	**23.67 °C**	**296.82 K**			
CSID	21111776	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	151.5929	**H bond donors**	0	**ACD/LogP**	2.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.19 g/cm^3



SMILES	Clc1ccccc1CC#N
STD InChIKey	MRDUURPIPLIGQX-UHFFFAOYAY

Melting Points

mp °C	source
24.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
23.00	Alfa Aesar
24.00	PHYSPROP

2-chloroethanol C2H5ClO[3, 19, 37, 59, 61, 64]

Compound Data

Melting point	**-66.25 °C**	**206.90 K**			
CSID	21106015	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	80.5135	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	ClCCO				
STD InChIKey	SZIFAVKTNFCBPC-UHFFFAOYAF				

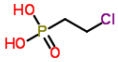
Melting Points

mp °C	source
-63.00	Alfa Aesar
-67.00	Fisher
-67.50	NIST Web Book
-67.50	PHYSPROP
	Values not used in calculating the average melting point
159.50	Chemical Book[1]
-89.00	Oxford University MSDS[2]

1. clearly out of range JCB
2. clearly out of range (4 NIST values) JCB

2-chloroethylphosphonic acid C2H6ClO3P[3, 64, 64]

Compound Data



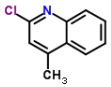
Melting point	**72.83 °C**	**345.98 K**			
CSID	26031	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	144.494	**H bond donors**	2	**ACD/LogP**	-1.42
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.57 g/cm^3
SMILES	ClCCP(=O)(O)O				
STD InChIKey	UDPGUMQDCGORJQ-UHFFFAOYAQ				

Melting Points

mp °C	source
70.00	Alfa Aesar
74.50	PHYSPROP
74.00	PHYSPROP

2-chlorolepidine C10H8ClN[3, 47, 64]

Compound Data

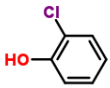


Melting point	**56.95 °C**	**330.10 K**			
CSID	62656	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.6302	**H bond donors**	0	**ACD/LogP**	3.17
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3
SMILES	Clc1nc2ccccc2c(c1)C				
STD InChIKey	PFEIMKNQOIFKSW-UHFFFAOYAZ				

Melting Points

mp °C	source
55.00	Alfa Aesar
56.85	IUCr
59.00	PHYSPROP

2-chlorophenol C6H5ClO[2, 3, 61, 64]



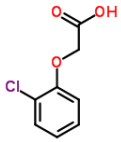
Compound Data

Melting point	**8.20 °C**	**281.35 K**			
CSID	13837686	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	128.5563	**H bond donors**	1	**ACD/LogP**	2.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Oc1ccccc1Cl				
STD InChIKey	ISPYQTSUDJAMAB-UHFFFAOYAM				

Melting Points

mp °C	source
8.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
8.00	Alfa Aesar
7.00	Oxford University MSDS
9.80	PHYSPROP

2-chlorophenoxyacetic acid C8H7ClO3[3, 64]



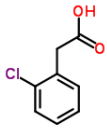
Compound Data

Melting point	**149.25 °C**	**422.40 K**			
CSID	11475	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	186.5924	**H bond donors**	1	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.37 g/cm^3
SMILES	Clc1ccccc1OCC(=O)O				
STD InChIKey	OPQYFNRLWBWCST-UHFFFAOYAU				

Melting Points

mp °C	source
150.00	Alfa Aesar
148.50	PHYSPROP

2-chlorophenylacetic acid C8H7ClO2[2, 3]



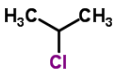
Compound Data

Melting point	**95.50 °C**	**368.65 K**			
CSID	16208	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	170.593	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	Clc1ccccc1CC(=O)O				
STD InChIKey	IUJAAIZKRJJZGQ-UHFFFAOYAB				

Melting Points

mp °C	source
95.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
96.00	Alfa Aesar

2-chloropropane C3H7Cl[3, 31, 61, 64]



Compound Data

Melting point	**-117.30 °C**	**155.85 K**			
CSID	6121	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	78.5407	**H bond donors**	0	**ACD/LogP**	1.85
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	ClC(C)C				
STD InChIKey	ULYZAYCEDJDHCC-UHFFFAOYAB				

Melting Points

mp °C	source
-117.00	Alfa Aesar
-117.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-118.00	Oxford University MSDS
-117.20	PHYSPROP

2-chloropropene C3H5Cl[3, 64]

Compound Data

Melting point	**-137.70 °C**	**135.45 K**			
CSID	10730	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	76.5248	**H bond donors**	0	**ACD/LogP**	1.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.91 g/cm^3
SMILES	Cl/C(=C)C				
STD InChIKey	PNLQPWWBHXMFCA-UHFFFAOYAD				

Melting Points

mp °C	source
-138.00	Alfa Aesar
-137.40	PHYSPROP

2-chloropyridine C5H4ClN[3, 64]

Compound Data

Melting point	**-46.25 °C**	**226.90 K**			
CSID	7689	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	113.545	**H bond donors**	0	**ACD/LogP**	1.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	Clc1ncccc1				
STD InChIKey	OKDGRDCXVWSXDC-UHFFFAOYAI				

Melting Points

mp °C	source
-46.00	Alfa Aesar
-46.50	PHYSPROP

2-chloropyrimidine C4H3ClN2[3, 64]

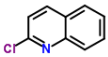
Compound Data

Melting point	**66.50 °C**	**339.65 K**			
CSID	66996	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.533	**H bond donors**	0	**ACD/LogP**	0.36
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.30 g/cm^3
SMILES	c1cnc(nc1)Cl				
STD InChIKey	UNCQVRBWJWWJBF-UHFFFAOYAB				

Melting Points

mp °C	source
66.00	Alfa Aesar
67.00	PHYSPROP

2-chloroquinoline C9H6ClN[3, 64]



Compound Data

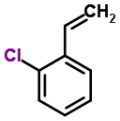
Melting point	**37.00 °C**	**310.15 K**			
CSID	11434	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.6036	**H bond donors**	0	**ACD/LogP**	2.71
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	Clc1nc2ccccc2cc1				
STD InChIKey	OFUFXTHGZWIDDB-UHFFFAOYAC				

Melting Points

mp °C	source
36.00	Alfa Aesar
38.00	PHYSPROP

2-chlorostyrene C8H7Cl[3, 64]

Compound Data



Melting point	**-63.05 °C**	**210.10 K**			
CSID	14205	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	138.5942	**H bond donors**	0	**ACD/LogP**	3.55
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	C=Cc1ccccc1Cl				
STD InChIKey	ISRGONDNXBCDBM-UHFFFAOYAD				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-63.10	PHYSPROP

2-chlorothiophene C4H3ClS[3, 64]

Compound Data

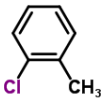
Melting point	**-71.95 °C**	**201.20 K**			
CSID	7027	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.5846	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.30 g/cm^3
SMILES	Clc1sccc1				
STD InChIKey	GSFNQBFZFXUTBN-UHFFFAOYAH				

Melting Points

mp °C	source
-72.00	Alfa Aesar
-71.90	PHYSPROP

2-chlorotoluene C7H7Cl[3, 31, 64]

Compound Data



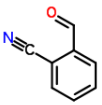
Melting point	**-35.53 °C**	**237.62 K**			
CSID	13875281	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	126.5835	**H bond donors**	0	**ACD/LogP**	3.36
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	Cc1ccccc1Cl				
STD InChIKey	IBSQPLPBRSHTTG-UHFFFAOYAU				

Melting Points

mp °C	source
-36.00	Alfa Aesar
-35.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-35.60	PHYSPROP

2-cyanobenzaldehyde C8H5NO[3, 7]

Compound Data



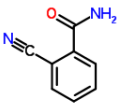
Melting point	**106.00 °C**	**379.15 K**			
CSID	91446	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	131.1314	**H bond donors**	0	**ACD/LogP**	1.45
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	N#Cc1ccccc1C=O				
STD InChIKey	QVTPWONEVZJCCS-UHFFFAOYAO				

Melting Points

mp °C	source
104.00	Alfa Aesar
108.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

2-cyanobenzamide C8H6N2O[3, 7]

Compound Data



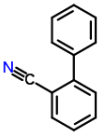
Melting point	**172.50 °C 445.65 K**				
CSID	65715	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	146.146	**H bond donors**	2	**ACD/LogP**	-0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	N#Cc1ccccc1C(=O)N				
STD InChIKey	STQPCKPKAIRSEL-UHFFFAOYAY				

Melting Points

mp °C	source
173.00	Alfa Aesar
172.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

2-cyanobiphenyl C13H9N[7, 64]

Compound Data



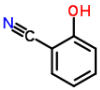
Melting point	**39.50 °C 312.65 K**				
CSID	124512	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	179.2173	**H bond donors**	0	**ACD/LogP**	3.18
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	N#Cc2ccccc2c1ccccc1				
STD InChIKey	WLPATYNQCGVFFH-UHFFFAOYAZ				

Melting Points

mp °C	source
38.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
41.00	PHYSPROP

2-cyanophenol C7H5NO[2, 3, 61, 64]

Compound Data



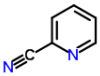
Melting point	**94.88 °C 368.02 K**				
CSID	11413	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	119.1207	**H bond donors**	1	**ACD/LogP**	1.61
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	N#Cc1ccccc1O				
STD InChIKey	CHZCERSEMVWNHL-UHFFFAOYAQ				

Melting Points

mp °C	source
94.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
94.00	Alfa Aesar
93.50	Oxford University MSDS
98.00	PHYSPROP

2-cyanopyridine C6H4N2[3, 64]

Compound Data



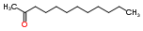
Melting point	**28.00 °C 301.15 K**				
CSID	7241	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	104.1094	**H bond donors**	0	**ACD/LogP**	0.51
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.12 g/cm^3
SMILES	N#Cc1ncccc1				
STD InChIKey	FFNVQNRYTPFDDP-UHFFFAOYAF				

Melting Points

mp °C	source
27.00	Alfa Aesar
29.00	PHYSPROP

2-dodecanone C12H24O[3, 4, 64]

Compound Data



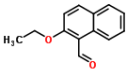
Melting point	**20.33 °C**	**293.48 K**			
CSID	21153	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.3184	**H bond donors**	0	**ACD/LogP**	4.62
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.82 g/cm^3
SMILES	O=C(CCCCCCCCCC)C				
STD InChIKey	LSKONYYRONEBKA-UHFFFAOYAA				

Melting Points

mp °C	source
19.00	Alfa Aesar
21.00	American Petroleum Institute. Research Project 44; Selected ...
21.00	PHYSPROP

2-ethoxy-1-naphthaldehyde C13H12O2[3, 64]

Compound Data



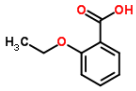
Melting point	**113.50 °C**	**386.65 K**			
CSID	79481	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.2332	**H bond donors**	0	**ACD/LogP**	3.48
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	O=Cc1c2c(ccc1OCC)cccc2				
STD InChIKey	IMNKQTWVJHODOS-UHFFFAOYAP				

Melting Points

mp °C	source
112.00	Alfa Aesar
115.00	PHYSPROP

2-ethoxybenzoic acid C9H10O3[3, 64]

Compound Data



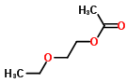
Melting point	**20.35 °C**	**293.50 K**			
CSID	60586	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	2.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)c1ccccc1OCC				
STD InChIKey	XDZMPRGFOOFSBL-UHFFFAOYAO				

Melting Points

mp °C	source
20.00	Alfa Aesar
20.70	PHYSPROP

2-ethoxyethyl acetate C6H12O3[2, 3, 61, 64]

Compound Data



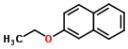
Melting point	**-61.67 °C**	**211.47 K**			
CSID	13839109	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	132.1577	**H bond donors**	0	**ACD/LogP**	0.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.96 g/cm^3
SMILES	CC(=O)OCCOCC				
STD InChIKey	SVONRAPFKPVNKG-UHFFFAOYAH				

Melting Points

mp °C	source

-61.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-62.00	Alfa Aesar
-62.00	Oxford University MSDS
-61.70	PHYSPROP

2-ethoxynaphthalene C12H12O[3, 64]



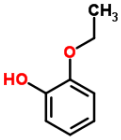
Compound Data

Melting point	**36.75 °C**	**309.90 K**			
CSID	6862	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	172.2231	**H bond donors**	0	**ACD/LogP**	3.90
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	O(c2ccc1c(cccc1)c2)CC				
STD InChIKey	GUMOJENFFHZAFP-UHFFFAOYAD				

Melting Points

mp °C	source
36.00	Alfa Aesar
37.50	PHYSPROP

2-ethoxyphenol C8H10O2[3, 64]



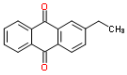
Compound Data

Melting point	**27.50 °C**	**300.65 K**			
CSID	60121	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	1	**ACD/LogP**	1.72
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	O(c1ccccc1O)CC				
STD InChIKey	MOEFFSWKSMRFRQ-UHFFFAOYAO				

Melting Points

mp °C	source
26.00	Alfa Aesar
29.00	PHYSPROP

2-ethyl anthraquinone C16H12O2[3, 61, 64]



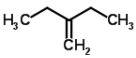
Compound Data

Melting point	**109.17 °C**	**382.32 K**			
CSID	6514	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	236.2653	**H bond donors**	0	**ACD/LogP**	4.38
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	O=C2c1c(cccc1)C(=O)c3c2ccc(c3)CC				
STD InChIKey	SJEBAWHUJDUKQK-UHFFFAOYAW				

Melting Points

mp °C	source
109.00	Alfa Aesar
109.00	Oxford University MSDS
109.50	PHYSPROP

2-ethyl-1-butene C6H12[3, 4, 64]



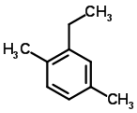
Compound Data

Melting point	**-131.83 °C**	**141.32 K**			
CSID	12430	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.69 g/cm^3
SMILES	C=C(/CC)CC				
STD InChIKey	RYKZRKKEYSRDNF-UHFFFAOYAG				

Melting Points

mp °C	source
-132.00	Alfa Aesar
-132.00	American Petroleum Institute. Research Project 44; Selected ...
-131.50	PHYSPROP

2-ethyl-1,4-dimethylbenzene C10H14[4, 64]



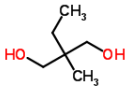
Compound Data

Melting point	**-53.85 °C**	**219.30 K**			
CSID	14888	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1c(ccc(c1CC)C)C				
STD InChIKey	AXIUBBVSOWPLDA-UHFFFAOYAU				

Melting Points

mp °C	source
-54.00	American Petroleum Institute. Research Project 44; Selected ...
-53.70	PHYSPROP

2-ethyl-2-methyl-1,3-propanediol C6H14O2[2, 64]



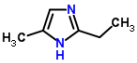
Compound Data

Melting point	**42.15 °C**	**315.30 K**			
CSID	59556	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1742	**H bond donors**	2	**ACD/LogP**	0.19
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	0.96 g/cm^3
SMILES	OCC(C)(CC)CO				
STD InChIKey	VNAWKNVDKFZFSU-UHFFFAOYAD				

Melting Points

mp °C	source
44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
40.30	PHYSPROP

2-ethyl-4-methylimidazole C6H10N2[3, 64]



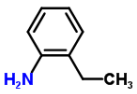
Compound Data

Melting point	**48.75 °C**	**321.90 K**			
CSID	63447	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	110.157	**H bond donors**	1	**ACD/LogP**	0.62
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	n1cc(nc1CC)C				
STD InChIKey	ULKLGIFJWFIQFF-UHFFFAOYAC				

Melting Points

mp °C	source
47.00	Alfa Aesar
50.50	PHYSPROP

2-ethylaniline C8H11N[2, 3, 64]



Compound Data

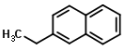
Melting point	**-45.83 °C**	**227.32 K**			
CSID	13860641	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	CCc1ccccc1N				
STD InChIKey	MLPVBIWIRCKMJV-UHFFFAOYAS				

Melting Points

mp °C	source

-44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-47.00	Alfa Aesar
-46.50	PHYSPROP

2-ethylnaphthalene C12H12[59, 59, 61, 64]



Compound Data

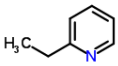
Melting point	**-7.40 °C**	**265.75 K**			
CSID	13063	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	156.2237	**H bond donors**	0	**ACD/LogP**	4.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	CCc1ccc2ccccc2c1				
STD InChIKey	RJTJVVYSTUQWNI-UHFFFAOYAX				

Melting Points

mp °C	source
-7.45	NIST Web Book
-7.35	NIST Web Book
-7.40	PHYSPROP
	Values not used in calculating the average melting point
34.85	NIST Web Book[1]
-70.00	Oxford University MSDS[2]

1. clearly out of range JCB
2. clearly out of range JCB

2-ethylpyridine C7H9N[3, 64]



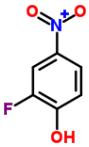
Compound Data

Melting point	**-63.05 °C**	**210.10 K**			
CSID	7242	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	0	**ACD/LogP**	1.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.93 g/cm^3
SMILES	n1ccccc1CC				
STD InChIKey	NRGGMCIBEHEAIL-UHFFFAOYAU				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-63.10	PHYSPROP

2-fluoro-4-nitrophenol C6H4FNO3[3, 64]



Compound Data

Melting point	**120.00 °C**	**393.15 K**			
CSID	9442	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	157.0993	**H bond donors**	1	**ACD/LogP**	1.70
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.51 g/cm^3
SMILES	Fc1cc([N+]([O-])=O)ccc1O				
STD InChIKey	ORPHLVJBJOCHBR-UHFFFAOYAU				

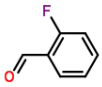
Melting Points

mp °C	source
119.00	Alfa Aesar
121.00	PHYSPROP

2-fluorobenzaldehyde C7H5FO[3, 64]

Compound Data

Melting point	**-44.75 °C**	**228.40 K**			
CSID	21106521	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	124.1124	**H bond donors**	0	**ACD/LogP**	1.79



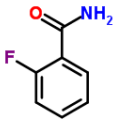
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	O=Cc1ccccc1F				
STD InChIKey	ZWDVQMVZZYIAHO-UHFFFAOYAA				

Melting Points

mp °C	source
-45.00	Alfa Aesar
-44.50	PHYSPROP

2-fluorobenzamide C7H6FNO[3, 64]

Compound Data



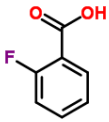
Melting point	**117.00 °C**	**390.15 K**			
CSID	61279	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	139.127	**H bond donors**	2	**ACD/LogP**	0.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	O=C(c1ccccc1F)N				
STD InChIKey	KGGHWIKBOIQEAJ-UHFFFAOYAW				

Melting Points

mp °C	source
116.00	Alfa Aesar
118.00	PHYSPROP

2-fluorobenzoic acid C7H5FO2[3, 64]

Compound Data



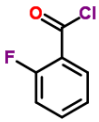
Melting point	**125.25 °C**	**398.40 K**			
CSID	9547	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	140.1118	**H bond donors**	1	**ACD/LogP**	1.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)c1ccccc1F				
STD InChIKey	NSTREUWFTAOOKS-UHFFFAOYAK				

Melting Points

mp °C	source
124.00	Alfa Aesar
126.50	PHYSPROP

2-fluorobenzoyl chloride C7H4ClFO[3, 64]

Compound Data



Melting point	**4.50 °C**	**277.65 K**			
CSID	9425	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	158.5575	**H bond donors**	0	**ACD/LogP**	1.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	O=C(Cl)c1ccccc1F				
STD InChIKey	RAAGZOYMEQDCTD-UHFFFAOYAQ				

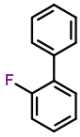
Melting Points

mp °C	source
5.00	Alfa Aesar
4.00	PHYSPROP

2-fluorobiphenyl C12H9F[3, 61, 64]

Compound Data

Melting point	**73.67 °C**	**346.82 K**			
CSID	60900	**H bond acceptors**	0	**Rule of 5 violations**	0



Molecular weight	172.1983	**H bond donors**	0	**ACD/LogP**	4.48
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	Fc2ccccc2c1ccccc1				
STD InChIKey	KLECYOQFQXJYBC-UHFFFAOYAW				

Melting Points

mp °C	source
74.00	Alfa Aesar
73.50	Oxford University MSDS
73.50	PHYSPROP

2-fluoroethanol C2H5FO[3, 64]

Compound Data

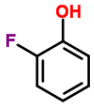
Melting point	**-26.70 °C**	**246.45 K**			
CSID	9354	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	64.0589	**H bond donors**	1	**ACD/LogP**	-0.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	FCCO				
STD InChIKey	GGDYAKVUZMZKRV-UHFFFAOYAT				

Melting Points

mp °C	source
-27.00	Alfa Aesar
-26.40	PHYSPROP

2-fluorophenol C6H5FO[3, 61, 64]

Compound Data



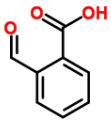
Melting point	**15.37 °C**	**288.52 K**			
CSID	9326	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	112.1017	**H bond donors**	1	**ACD/LogP**	1.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	Fc1ccccc1O				
STD InChIKey	HFHFGHLXUCOHLN-UHFFFAOYAV				

Melting Points

mp °C	source
15.00	Alfa Aesar
15.00	Oxford University MSDS
16.10	PHYSPROP

2-formylbenzoic acid C8H6O3[2, 3, 64]

Compound Data

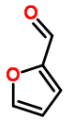


Melting point	**98.00 °C**	**371.15 K**			
CSID	8099	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1314	**H bond donors**	1	**ACD/LogP**	0.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	c1ccc(c(c1)C=O)C(=O)O				
STD InChIKey	DYNFCHNNOHNJFG-UHFFFAOYAX				

Melting Points

mp °C	source
97.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
99.00	Alfa Aesar
98.00	PHYSPROP

2-furaldehyde C5H4O2[3, 35, 61, 64]



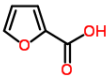
Compound Data

Melting point	**-37.15 °C**	**236.00 K**			
CSID	13863629	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	96.0841	**H bond donors**	0	**ACD/LogP**	0.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	c1cc(oc1)C=O				
STD InChIKey	HYBBIBNJHNGZAN-UHFFFAOYAD				

Melting Points

mp °C	source
-38.00	Alfa Aesar
-36.50	EPISuite-ChemSpider
-36.00	Oxford University MSDS
-38.10	PHYSPROP

2-furoic acid C5H4O3[3, 35, 64]



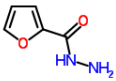
Compound Data

Melting point	**132.33 °C**	**405.48 K**			
CSID	10251740	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	112.0835	**H bond donors**	1	**ACD/LogP**	0.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	OC(=O)c1ccco1				
STD InChIKey	SMNDYUVBFMFKNZ-UHFFFAOYAH				

Melting Points

mp °C	source
130.00	Alfa Aesar
133.50	EPISuite-ChemSpider
133.50	PHYSPROP

2-furoic acid hydrazide C5H6N2O2[3, 48]



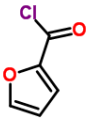
Compound Data

Melting point	**79.50 °C**	**352.65 K**			
CSID	17687	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	126.1133	**H bond donors**	3	**ACD/LogP**	-0.59
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.26 g/cm^3
SMILES	O=C(NN)c1occc1				
STD InChIKey	SKTSVWWOAIAIKI-UHFFFAOYAV				

Melting Points

mp °C	source
79.00	Alfa Aesar
80.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2-furoyl chloride C5H3ClO2[3, 64, 64]



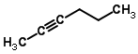
Compound Data

Melting point	**-1.67 °C**	**271.48 K**			
CSID	13861158	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.5291	**H bond donors**	0	**ACD/LogP**	1.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	ClC(=O)c1ccco1				
STD InChIKey	OFTKFKYVSBNYEC-UHFFFAOYAN				

Melting Points

mp °C	source
-1.00	Alfa Aesar
-2.00	PHYSPROP
-2.00	PHYSPROP

2-hexyne C6H10[3, 4, 64]



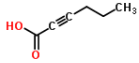
Compound Data

Melting point	**-89.87 °C**	**183.28 K**			
CSID	31016	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.74 g/cm^3
SMILES	C(#CCCC)C				
STD InChIKey	MELUCTCJOARQQG-UHFFFAOYAT				

Melting Points

mp °C	source
-90.00	Alfa Aesar
-90.00	American Petroleum Institute. Research Project 44; Selected ...
-89.60	PHYSPROP

2-hexynoic acid C6H8O2[3, 64]



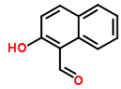
Compound Data

Melting point	**26.00 °C**	**299.15 K**			
CSID	287294	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	112.1265	**H bond donors**	1	**ACD/LogP**	1.92
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	O=C(C#CCCC)O				
STD InChIKey	AKYAUBWOTZJUBI-UHFFFAOYAU				

Melting Points

mp °C	source
25.00	Alfa Aesar
27.00	PHYSPROP

2-hydroxy-1-naphthaldehyde C11H8O2[3, 64]



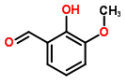
Compound Data

Melting point	**81.00 °C**	**354.15 K**			
CSID	12291	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.18	**H bond donors**	1	**ACD/LogP**	2.84
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.29 g/cm^3
SMILES	O=Cc1c2c(ccc1O)cccc2				
STD InChIKey	NTCCNERMXRIPTR-UHFFFAOYAU				

Melting Points

mp °C	source
79.00	Alfa Aesar
83.00	PHYSPROP

2-hydroxy-3-methoxybenzaldehyde C8H8O3[3, 35, 61, 64]



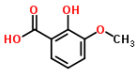
Compound Data

Melting point	**42.75 °C**	**315.90 K**			
CSID	21105848	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.40
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	Oc1c(cccc1OC)C=O				
STD InChIKey	JJVNINGBHGBWJH-UHFFFAOYAB				

Melting Points

mp °C	source
41.00	Alfa Aesar
44.50	EPISuite-ChemSpider
41.00	Oxford University MSDS
44.50	PHYSPROP

2-hydroxy-3-methoxybenzoic acid $C_8H_8O_4$[3, 64]



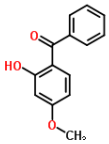
Compound Data

Melting point	**151.50 °C**	**424.65 K**			
CSID	63328	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	2	**ACD/LogP**	1.98
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.35 g/cm^3
SMILES	O=C(O)c1cccc(OC)c1O				
STD InChIKey	AUZQQIPZESHNMG-UHFFFAOYAG				

Melting Points

mp °C	source
152.00	Alfa Aesar
151.00	PHYSPROP

2-hydroxy-4-methoxybenzophenone $C_{14}H_{12}O_3$[3, 64]



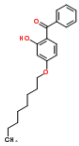
Compound Data

Melting point	**64.75 °C**	**337.90 K**			
CSID	4471	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	228.2433	**H bond donors**	1	**ACD/LogP**	3.64
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	O=C(c1ccc(OC)cc1O)c2ccccc2				
STD InChIKey	DXGLGDHPHMLXJC-UHFFFAOYAX				

Melting Points

mp °C	source
64.00	Alfa Aesar
65.50	PHYSPROP

2-hydroxy-4-octyloxybenzophenone $C_{21}H_{26}O_3$[3, 64]



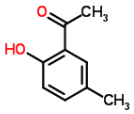
Compound Data

Melting point	**48.25 °C**	**321.40 K**			
CSID	15020	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	326.4293	**H bond donors**	1	**ACD/LogP**	7.36
Phase 25 °C	solid	**Rotatable bonds**	11	**Predicted density**	1.07 g/cm^3
SMILES	O=C(c1ccc(OCCCCCCCC)cc1O)c2ccccc2				
STD InChIKey	QUAMTGJKVDWJEQ-UHFFFAOYAM				

Melting Points

mp °C	source
48.00	Alfa Aesar
48.50	PHYSPROP

2-hydroxy-5-methylacetophenone $C_9H_{10}O_2$[3, 64]



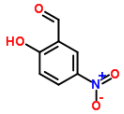
Compound Data

Melting point	**48.50 °C**	**321.65 K**			
CSID	14340	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	O=C(c1cc(ccc1O)C)C				
STD InChIKey	YNPDFBFVMJNGKZ-UHFFFAOYAB				

Melting Points

mp °C	source
47.00	Alfa Aesar
50.00	PHYSPROP

2-hydroxy-5-nitrobenzaldehyde $C_7H_5NO_4$[3, 64]



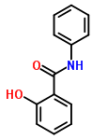
Compound Data

Melting point	**127.00 °C**	**400.15 K**			
CSID	60173	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	167.1189	**H bond donors**	1	**ACD/LogP**	2.08
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.50 g/cm^3
SMILES	O=Cc1cc(ccc1O)[N+](=O)[O-]=O				
STD InChIKey	IHFRMUGEILMHNU-UHFFFAOYAV				

Melting Points

mp °C	source
125.00	Alfa Aesar
129.00	PHYSPROP

2-hydroxy-N-phenylbenzamide C13H11NO2[3, 64]



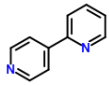
Compound Data

Melting point	**136.75 °C**	**409.90 K**			
CSID	6610	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	213.2319	**H bond donors**	2	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.28 g/cm^3
SMILES	O=C(c1ccccc1O)Nc2ccccc2				
STD InChIKey	WKEDVNSFRWHDNR-UHFFFAOYAI				

Melting Points

mp °C	source
137.00	Alfa Aesar
136.50	PHYSPROP

2-hydroxyacetophenone C10H8N2[3, 64]



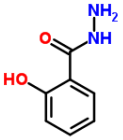
Compound Data

Melting point	**61.25 °C**	**334.40 K**			
CSID	61763	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.1839	**H bond donors**	0	**ACD/LogP**	1.24
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	n2ccc(c1ncccc1)cc2				
STD InChIKey	RMHQDKYZXJVCME-UHFFFAOYAG				

Melting Points

mp °C	source
61.00	Alfa Aesar
61.50	PHYSPROP

2-hydroxybenzhydrazide C7H8N2O2[3, 64]



Compound Data

Melting point	**148.25 °C**	**421.40 K**			
CSID	13048	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	4	**ACD/LogP**	0.60
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	O=C(c1ccccc1O)NN				
STD InChIKey	XSXYESVZDBAKKT-UHFFFAOYAC				

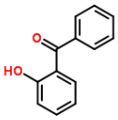
Melting Points

mp °C	source
148.00	Alfa Aesar
148.50	PHYSPROP

2-hydroxybenzophenone C13H10O2[3, 64]

Compound Data

Melting point	**39.50 °C**	**312.65 K**



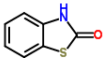
CSID	8045	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2173	**H bond donors**	1	**ACD/LogP**	3.47
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.19 g/cm^3
SMILES	O=C(c1ccccc1O)c2ccccc2				
STD InChIKey	HJIAMFHSAAEUKR-UHFFFAOYAQ				

Melting Points

mp °C	source
39.00	Alfa Aesar
40.00	PHYSPROP

2-hydroxybenzothiazole C7H5NOS[3, 64]

Compound Data



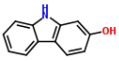
Melting point	**138.50 °C**	**411.65 K**			
CSID	13036	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	151.1857	**H bond donors**	1	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.37 g/cm^3
SMILES	O=C2Sc1ccccc1N2				
STD InChIKey	YEDUAINPPJYDJZ-UHFFFAOYAF				

Melting Points

mp °C	source
138.00	Alfa Aesar
139.00	PHYSPROP

2-hydroxycarbazole C12H9NO[3, 64]

Compound Data



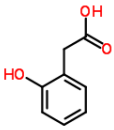
Melting point	**271.75 °C**	**544.90 K**			
CSID	84451	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	183.206	**H bond donors**	2	**ACD/LogP**	2.98
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	Oc3ccc2c1ccccc1nc2c3				
STD InChIKey	GWPGDZPXOZATKL-UHFFFAOYAN				

Melting Points

mp °C	source
272.00	Alfa Aesar
271.50	PHYSPROP

2-hydroxyphenylacetic acid C8H8O3[3, 48, 64]

Compound Data



Melting point	**147.67 °C**	**420.82 K**			
CSID	11476	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)Cc1ccccc1O				
STD InChIKey	CCVYRRGZDBSHFU-UHFFFAOYAL				

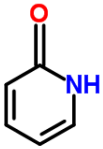
Melting Points

mp °C	source
146.00	Alfa Aesar
149.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
148.00	PHYSPROP

2-hydroxypyridine C5H5NO[3, 64, 64]

Compound Data

Melting point	**107.53 °C**	**380.68 K**



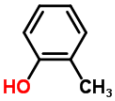
CSID	8537	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	95.0993	**H bond donors**	1	**ACD/LogP**	-0.58
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c1cc[nH]c(=O)c1				
STD InChIKey	UBQKCCHYAOITMY-UHFFFAOYAK				

Melting Points

mp °C	source
107.00	Alfa Aesar
107.80	PHYSPROP
107.80	PHYSPROP

2-hydroxytoluene C7H8O[3, 31, 61, 64]

Compound Data



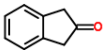
Melting point	**31.45 °C**	**304.60 K**			
CSID	13835772	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	108.1378	**H bond donors**	1	**ACD/LogP**	1.96
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	Cc1ccccc1O				
STD InChIKey	QWVGKYWNOKOFNN-UHFFFAOYAS				

Melting Points

mp °C	source
32.00	Alfa Aesar
31.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
33.00	Oxford University MSDS
29.80	PHYSPROP

2-indanone C9H8O[3, 64]

Compound Data



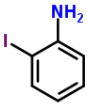
Melting point	**56.50 °C**	**329.65 K**			
CSID	11488	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	132.1592	**H bond donors**	0	**ACD/LogP**	1.23
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.15 g/cm^3
SMILES	O=C2Cc1ccccc1C2				
STD InChIKey	UMJJFEIKYGFCAT-UHFFFAOYAK				

Melting Points

mp °C	source
54.00	Alfa Aesar
59.00	PHYSPROP

2-iodaniline C6H6IN[2, 3, 64]

Compound Data

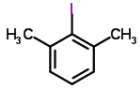


Melting point	**56.50 °C**	**329.65 K**			
CSID	11500	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	219.023	**H bond donors**	2	**ACD/LogP**	2.30
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.92 g/cm^3
SMILES	Ic1ccccc1N				
STD InChIKey	UBPDKIDWEADHPP-UHFFFAOYAT				

Melting Points

mp °C	source
58.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
56.50	PHYSPROP

2-iodo-1,3-dimethylbenzene C8H9I[7, 64]



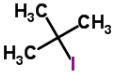
Compound Data

Melting point	**11.10 °C**	**284.25 K**			
CSID	62314	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	232.0615	**H bond donors**	0	**ACD/LogP**	4.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.61 g/cm^3
SMILES	Ic1c(cccc1C)C				
STD InChIKey	QTUGGVBKWIYQSS-UHFFFAOYAW				

Melting Points

mp °C	source
11.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
11.20	PHYSPROP

2-iodo-2-methylpropane C4H9I[2, 3, 61, 64]



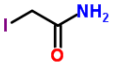
Compound Data

Melting point	**-38.05 °C**	**235.10 K**			
CSID	10733	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	184.0187	**H bond donors**	0	**ACD/LogP**	2.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.62 g/cm^3
SMILES	IC(C)(C)C				
STD InChIKey	ANGGPYSFTXVERY-UHFFFAOYAE				

Melting Points

mp °C	source
-38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-38.00	Alfa Aesar
-38.00	Oxford University MSDS
-38.20	PHYSPROP

2-iodoacetamide C2H4INO[3, 61, 64]



Compound Data

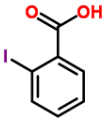
Melting point	**94.00 °C**	**367.15 K**			
CSID	3596	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	184.9637	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.28 g/cm^3
SMILES	C(C(=O)N)I				
STD InChIKey	PGLTVOMIXTUURA-UHFFFAOYAE				

Melting Points

mp °C	source
93.50	Alfa Aesar
94.00	Oxford University MSDS
94.50	PHYSPROP
	Values not used in calculating the average melting point
-94.00	Alfa Aesar[1]

1. sign inversion JCB

2-iodobenzoic acid C7H5IO2[2, 3, 61, 64]



Compound Data

Melting point	**162.38 °C**	**435.52 K**			
CSID	6675	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	248.0179	**H bond donors**	1	**ACD/LogP**	2.16
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.00 g/cm^3
SMILES	O=C(O)c1ccccc1I				
STD InChIKey	CJNZAXGUTKBIHP-UHFFFAOYAT				

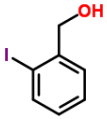
Melting Points

mp °C	source
162.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

162.00	Alfa Aesar
162.50	Oxford University MSDS
163.00	PHYSPROP

2-iodobenzyl alcohol C7H7IO[2, 3, 64]

Compound Data



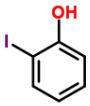
Melting point	**91.67 °C**	**364.82 K**			
CSID	96816	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	234.0343	**H bond donors**	1	**ACD/LogP**	2.07
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.87 g/cm^3
SMILES	Ic1ccccc1CO				
STD InChIKey	WZCXOBMFBKSSFA-UHFFFAOYAP				

Melting Points

mp °C	source
92.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
91.00	Alfa Aesar
92.00	PHYSPROP

2-iodophenol C6H5IO[3, 7, 56, 61, 64, 72]

Compound Data



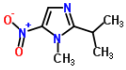
Melting point	**40.83 °C**	**313.98 K**			
CSID	10328	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	220.0078	**H bond donors**	1	**ACD/LogP**	2.65
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.00 g/cm^3
SMILES	Ic1ccccc1O				
STD InChIKey	KQDJTBPASNJQFQ-UHFFFAOYAN				

Melting Points

mp °C	source
40.00	Alfa Aesar
42.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
43.00	Merck Index
38.50	Oxford University MSDS
43.00	PHYSPROP
38.50	Sigma-Aldrich

2-isopropyl-1-methyl-5-nitroimidazole C7H11N3O2[64, 70]

Compound Data



Melting point	**60.50 °C**	**333.65 K**			
CSID	25097	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	169.1811	**H bond donors**	0	**ACD/LogP**	1.19
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	[O-][N+](=O)c1cnc(n1C)C(C)C				
STD InChIKey	NTAFJUSDNOSFFY-UHFFFAOYAB				

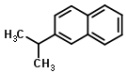
Melting Points

mp °C	source
60.00	PHYSPROP
61.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

2-isopropylnaphthalene C13H14[3, 64]

Compound Data

Melting point	**14.25 °C**	**287.40 K**			
CSID	15410	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	170.2503	**H bond donors**	0	**ACD/LogP**	4.79
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3



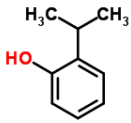
SMILES	c12ccccc1ccc(c2)C(C)C
STD InChIKey	TVYVQNHYIHAJTD-UHFFFAOYAA

Melting Points

mp °C	source
14.00	Alfa Aesar
14.50	PHYSPROP

2-isopropylphenol C9H12O[2, 2, 3, 64]

Compound Data



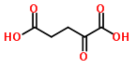
Melting point	**15.62 °C**	**288.77 K**			
CSID	6677	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	1	**ACD/LogP**	2.82
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	Oc1ccccc1C(C)C				
STD InChIKey	CRBJBYGJVIBWIY-UHFFFAOYAA				

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
15.00	Alfa Aesar
15.50	PHYSPROP

2-ketoglutaric acid C5H6O5[3, 35, 64]

Compound Data



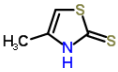
Melting point	**115.33 °C**	**388.48 K**			
CSID	50	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	146.0981	**H bond donors**	2	**ACD/LogP**	-1.43
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.50 g/cm^3
SMILES	O=C(O)C(=O)CCC(=O)O				
STD InChIKey	KPGXRSRHYNQIFN-UHFFFAOYAN				

Melting Points

mp °C	source
115.00	Alfa Aesar
115.50	EPISuite-ChemSpider
115.50	PHYSPROP

2-mercapto-4-methylthiazole C4H5NS2[3, 64]

Compound Data

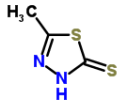


Melting point	**88.65 °C**	**361.80 K**			
CSID	1013221	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	131.2192	**H bond donors**	1	**ACD/LogP**	1.48
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.36 g/cm^3
SMILES	S=C1S\C=C(/N1)C				
STD InChIKey	NLHAIPFBNQZTMY-UHFFFAOYAK				

Melting Points

mp °C	source
88.00	Alfa Aesar
89.30	PHYSPROP

2-mercapto-5-methyl-1,3,4-thiadiazole C3H4N2S2[3, 48]



Compound Data

Melting point	**185.50 °C**	**458.65 K**			
CSID	1414905	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	132.2073	**H bond donors**	1	**ACD/LogP**	-0.26
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.58 g/cm^3
SMILES	S=C1S\C(=N/N1)C				
STD InChIKey	FPVUWZFFEGYCGB-UHFFFAOYAO				

Melting Points

mp °C	source
184.00	Alfa Aesar
187.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2-mercaptoimidazole C3H4N2S[3, 64]

Compound Data

Melting point	**227.25 °C**	**500.40 K**			
CSID	1013196	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1423	**H bond donors**	2	**ACD/LogP**	0.21
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.36 g/cm^3
SMILES	S=C1N\C=C/N1				
STD InChIKey	OXFSTTJBVAAALW-UHFFFAOYAJ				

Melting Points

mp °C	source
225.00	Alfa Aesar
229.50	PHYSPROP

2-mercaptothiazoline C3H5NS2[3, 64]

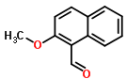
Compound Data

Melting point	**105.50 °C**	**378.65 K**			
CSID	2005898	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	119.2085	**H bond donors**	1	**ACD/LogP**	0.82
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.38 g/cm^3
SMILES	S=C1SCCN1				
STD InChIKey	WGJCBBASTRWVJL-UHFFFAOYAV				

Melting Points

mp °C	source
105.00	Alfa Aesar
106.00	PHYSPROP

2-methoxy-1-naphthaldehyde C12H10O2[3, 3]



Compound Data

Melting point	**83.50 °C**	**356.65 K**			
CSID	71672	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	0	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=Cc1c2c(ccc1OC)cccc2				
STD InChIKey	YIQGLTKAOHRZOL-UHFFFAOYAN				

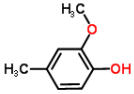
Melting Points

mp °C	source
84.00	Alfa Aesar
83.00	Alfa Aesar

2-methoxy-4-methylphenol C8H10O2[3, 64]

Compound Data

Melting point	**5.75 °C**	**278.90 K**



CSID	21105936	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	1	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.08 g/cm^3
SMILES	Oc1ccc(C)cc1OC				
STD InChIKey	PETRWTHZSKVLRE-UHFFFAOYAK				

Melting Points

mp °C	source
6.00	Alfa Aesar
5.50	PHYSPROP

2-methoxy-4-nitroaniline C7H8N2O3[3, 64]

Compound Data

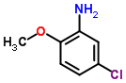
Melting point	**140.50 °C**	**413.65 K**			
CSID	7060	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	168.15	**H bond donors**	2	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	[O-][N+](=O)c1cc(OC)c(N)cc1				
STD InChIKey	GVBHRNIWBGTNQA-UHFFFAOYAF				

Melting Points

mp °C	source
140.00	Alfa Aesar
141.00	PHYSPROP

2-methoxy-5-chloroaniline C7H8ClNO[2, 3]

Compound Data



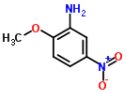
Melting point	**82.50 °C**	**355.65 K**			
CSID	60129	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	157.5975	**H bond donors**	2	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	Clc1cc(c(OC)cc1)N				
STD InChIKey	WBSMIPLNPSCJFS-UHFFFAOYAK				

Melting Points

mp °C	source
83.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
82.00	Alfa Aesar

2-methoxy-5-nitroaniline C7H8N2O3[3, 61, 64]

Compound Data



Melting point	**117.67 °C**	**390.82 K**			
CSID	7167	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	168.15	**H bond donors**	2	**ACD/LogP**	1.69
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	[O-][N+](=O)c1ccc(OC)c(N)c1				
STD InChIKey	NIPDVSLAMPAWTP-UHFFFAOYAL				

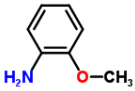
Melting Points

mp °C	source
117.00	Alfa Aesar
118.00	Oxford University MSDS
118.00	PHYSPROP

2-methoxyaniline C7H9NO[2, 3, 61, 64]

Compound Data

Melting point	**5.80 °C**	**278.95 K**



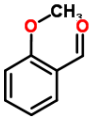
CSID	13860775	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	123.1525	**H bond donors**	2	**ACD/LogP**	1.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	Nc1ccccc1OC				
STD InChIKey	VMPITZXILSNTON-UHFFFAOYAW				

Melting Points

mp °C	source
6.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
6.00	Alfa Aesar
5.00	Oxford University MSDS
6.20	PHYSPROP

2-methoxybenzaldehyde C8H8O2[2, 3, 64]

Compound Data



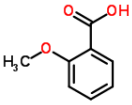
Melting point	**37.50 °C**	**310.65 K**			
CSID	21111781	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	0	**ACD/LogP**	1.72
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	COc1ccccc1C=O				
STD InChIKey	PKZJLOCLABXVMC-UHFFFAOYAR				

Melting Points

mp °C	source
38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
37.00	Alfa Aesar
37.50	PHYSPROP

2-methoxybenzoic acid C8H8O3[2, 3, 35, 64]

Compound Data



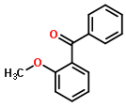
Melting point	**100.50 °C**	**373.65 K**			
CSID	10892	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	O=C(O)c1ccccc1OC				
STD InChIKey	ILUJQPXNXACGAN-UHFFFAOYAY				

Melting Points

mp °C	source
99.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
101.00	Alfa Aesar
101.00	EPISuite-ChemSpider
101.00	PHYSPROP

2-methoxybenzophenone C14H12O2[3, 64]

Compound Data

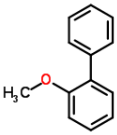


Melting point	**39.00 °C**	**312.15 K**			
CSID	68220	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	0	**ACD/LogP**	3.15
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=C(c1ccccc1OC)c2ccccc2				
STD InChIKey	CSUUDNFYSFENAE-UHFFFAOYAU				

Melting Points

mp °C	source
37.00	Alfa Aesar
41.00	PHYSPROP

2-methoxybiphenyl C13H12O[3, 7, 64]



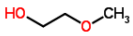
Compound Data

Melting point	**30.00 °C**	**303.15 K**			
CSID	6574	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.2338	**H bond donors**	0	**ACD/LogP**	3.64
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	O(c2ccccc2c1ccccc1)C				
STD InChIKey	NLWCWEGVNJVLAX-UHFFFAOYAF				

Melting Points

mp °C	source
30.00	Alfa Aesar
31.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
29.00	PHYSPROP

2-methoxyethanol C3H8O2[2, 3, 32, 61, 64]



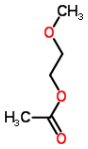
Compound Data

Melting point	**-85.04 °C**	**188.11 K**			
CSID	7728	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	76.0944	**H bond donors**	1	**ACD/LogP**	-0.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.93 g/cm^3
SMILES	OCCOC				
STD InChIKey	XNWFRZJHXBZDAG-UHFFFAOYAC				

Melting Points

mp °C	source
-85.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-85.00	Alfa Aesar
-85.10	DrugBank
-85.00	Oxford University MSDS
-85.10	PHYSPROP

2-methoxyethyl acetate C5H10O3[2, 64]



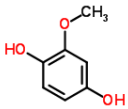
Compound Data

Melting point	**-65.05 °C**	**208.10 K**			
CSID	13864773	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	118.1311	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.98 g/cm^3
SMILES	CC(=O)OCCOC				
STD InChIKey	XLLIQLLCWZCATF-UHFFFAOYAF				

Melting Points

mp °C	source
-65.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-65.10	PHYSPROP

2-methoxyhydroquinone C7H8O3[3, 64]



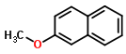
Compound Data

Melting point	**89.50 °C**	**362.65 K**			
CSID	63180	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	140.1366	**H bond donors**	2	**ACD/LogP**	0.71
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	COc1cc(ccc1O)O				
STD InChIKey	LAQYHRQFABOIFD-UHFFFAOYAC				

Melting Points

mp °C	source
89.00	Alfa Aesar
90.00	PHYSPROP

2-methoxynaphthalene C11H10O[3, 61, 64]



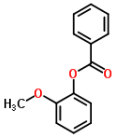
Compound Data

Melting point	**73.17 °C**	**346.32 K**			
CSID	6852	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	158.1965	**H bond donors**	0	**ACD/LogP**	3.36
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	O(c2ccc1c(cccc1)c2)C				
STD InChIKey	LUZDYPLAQQGJEA-UHFFFAOYAR				

Melting Points

mp °C	source
72.00	Alfa Aesar
74.00	Oxford University MSDS
73.50	PHYSPROP

2-methoxyphenyl benzoate C14H12O3[3, 64]



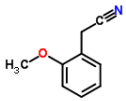
Compound Data

Melting point	**58.25 °C**	**331.40 K**			
CSID	61569	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	228.2433	**H bond donors**	0	**ACD/LogP**	3.52
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.16 g/cm^3
SMILES	O=C(Oc1ccccc1OC)c2ccccc2				
STD InChIKey	IZYQCDNLUPLXOO-UHFFFAOYAC				

Melting Points

mp °C	source
59.00	Alfa Aesar
57.50	PHYSPROP

2-methoxyphenylacetonitrile C9H9NO[2, 3, 64]



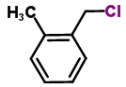
Compound Data

Melting point	**67.93 °C**	**341.08 K**			
CSID	73531	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	147.1739	**H bond donors**	0	**ACD/LogP**	1.36
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	N#CCc1ccccc1OC				
STD InChIKey	DWJKILXTMUGXOU-UHFFFAOYAZ				

Melting Points

mp °C	source
66.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
68.00	Alfa Aesar
69.80	PHYSPROP

2-methyl benzyl chloride C8H9Cl[3, 61]



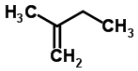
Compound Data

Melting point	**0.00 °C**	**273.15 K**			
CSID	21106134	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	140.6101	**H bond donors**	0	**ACD/LogP**	2.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	Cc1ccccc1CCl				
STD InChIKey	VQRBXYBBGHOGFT-UHFFFAOYAS				

Melting Points

mp °C	source
2.00	Alfa Aesar
-2.00	Oxford University MSDS

2-methyl-1-butene C_5H_{10}[3, 4, 61, 64]



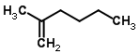
Compound Data

Melting point	**-137.38 °C**	**135.77 K**			
CSID	10766	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.92
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.66 g/cm^3
SMILES	C=C(/C)CC				
STD InChIKey	MHNNAWXXUZQSNM-UHFFFAOYAQ				

Melting Points

mp °C	source
-137.00	Alfa Aesar
-138.00	American Petroleum Institute. Research Project 44; Selected ...
-137.00	Oxford University MSDS
-137.50	PHYSPROP

2-methyl-1-hexene C_7H_{14}[4, 64]



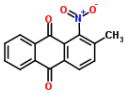
Compound Data

Melting point	**-102.90 °C**	**170.25 K**			
CSID	21073	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.71 g/cm^3
SMILES	C=C(/C)CCCC				
STD InChIKey	IRUDSQHLKGNCGF-UHFFFAOYAD				

Melting Points

mp °C	source
-103.00	American Petroleum Institute. Research Project 44; Selected ...
-102.80	PHYSPROP

2-methyl-1-nitroanthraquinone $C_{15}H_9NO_4$[48, 64]



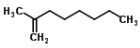
Compound Data

Melting point	**269.25 °C**	**542.40 K**			
CSID	29156	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	267.2363	**H bond donors**	0	**ACD/LogP**	3.67
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	[O-][N+](=O)c3c(ccc2C(=O)c1ccccc1C(=O)c23)C				
STD InChIKey	FYXKXZFTZBYYNP-UHFFFAOYAD				

Melting Points

mp °C	source
268.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
270.50	PHYSPROP

2-methyl-1-octene C_9H_{18}[4, 64]



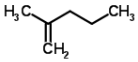
Compound Data

Melting point	**-77.90 °C**	**195.25 K**			
CSID	70705	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	126.2392	**H bond donors**	0	**ACD/LogP**	5.05
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.73 g/cm^3
SMILES	C=C(/C)CCCCCC				
STD InChIKey	FBEDQPGLIKZGIN-UHFFFAOYAQ				

Melting Points

mp °C	source
-78.00	American Petroleum Institute. Research Project 44; Selected ...
-77.80	PHYSPROP

2-methyl-1-pentene C_6H_{12}[3, 4, 64]



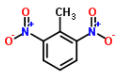
Compound Data

Melting point	**-135.90 °C**	**137.25 K**			
CSID	12446	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.69 g/cm^3
SMILES	C=C(/C)CCC				
STD InChIKey	WWUVJRULCWHUSA-UHFFFAOYAW				

Melting Points

mp °C	source
-136.00	Alfa Aesar
-136.00	American Petroleum Institute. Research Project 44; Selected ...
-135.70	PHYSPROP

2-methyl-1,3-dinitrobenzene $C_7H_6N_2O_4$[2, 3, 61, 64]



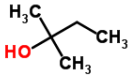
Compound Data

Melting point	**64.50 °C**	**337.65 K**			
CSID	11320	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	182.1335	**H bond donors**	0	**ACD/LogP**	1.98
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Cc1c(cccc1[N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	XTRDKALNCIHHNI-UHFFFAOYAI				

Melting Points

mp °C	source
65.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
62.00	Alfa Aesar
65.00	Oxford University MSDS
66.00	PHYSPROP

2-methyl-2-butanol $C_5H_{12}O$[3, 4, 64]



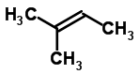
Compound Data

Melting point	**-9.70 °C**	**263.45 K**			
CSID	6165	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	1	**ACD/LogP**	1.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.81 g/cm^3
SMILES	OC(C)(C)CC				
STD InChIKey	MSXVEPNJUHWQHW-UHFFFAOYAG				

Melting Points

mp °C	source
-12.00	Alfa Aesar
-8.00	American Petroleum Institute. Research Project 44; Selected ...
-9.10	PHYSPROP

2-methyl-2-butene C_5H_{10}[3, 4, 61, 64]



Compound Data

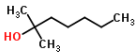
Melting point	**-133.93 °C**	**139.22 K**			
CSID	10113	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.92
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.67 g/cm^3
SMILES	C(=C(\C)C)\C				
STD InChIKey	BKOOMYPCSUNDGP-UHFFFAOYAE				

Melting Points

mp °C	source
-134.00	Alfa Aesar

-134.00	American Petroleum Institute. Research Project 44; Selected ...
-134.00	Oxford University MSDS
-133.70	PHYSPROP

2-methyl-2-heptanol C8H18O[64, 82]



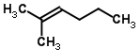
Compound Data

Melting point	**-50.20 °C**	**222.95 K**			
CSID	11741	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	130.2279	**H bond donors**	1	**ACD/LogP**	2.63
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.82 g/cm^3
SMILES	OC(C)(C)CCCCC				
STD InChIKey	ACBMYYVZWKYLIP-UHFFFAOYAE				

Melting Points

mp °C	source
-50.40	PHYSPROP
-50.00	Wilhoit R. C. Physical and Thermodynamic Properties of Aliph...

2-methyl-2-hexene C7H14[4, 4, 64]



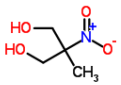
Compound Data

Melting point	**-130.13 °C**	**143.02 K**			
CSID	16689	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.98
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.71 g/cm^3
SMILES	C(=C\CCC)(\C)C				
STD InChIKey	BWEKDYGHDCHWEN-UHFFFAOYAR				

Melting Points

mp °C	source
-130.00	American Petroleum Institute. Research Project 44; Selected ...
-130.00	American Petroleum Institute. Research Project 44; Selected ...
-130.40	PHYSPROP

2-methyl-2-nitro-1,3-propanediol C4H9NO4[3, 64]



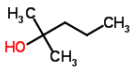
Compound Data

Melting point	**150.05 °C**	**423.20 K**			
CSID	6235	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	135.1186	**H bond donors**	2	**ACD/LogP**	0.14
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.32 g/cm^3
SMILES	[O-][N+](=O)C(C)(CO)CO				
STD InChIKey	LOTYADDQWWVBDJ-UHFFFAOYAT				

Melting Points

mp °C	source
150.00	Alfa Aesar
150.10	PHYSPROP

2-methyl-2-pentanol C6H14O[3, 4, 64]



Compound Data

Melting point	**-102.67 °C**	**170.48 K**			
CSID	11056	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	102.1748	**H bond donors**	1	**ACD/LogP**	1.57
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.82 g/cm^3
SMILES	OC(C)(C)CCC				
STD InChIKey	WFRBDWRZVBPBDO-UHFFFAOYAE				

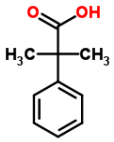
Melting Points

mp °C	source

-103.00	Alfa Aesar
-102.00	American Petroleum Institute. Research Project 44; Selected ...
-103.00	PHYSPROP

2-methyl-2-phenylpropanoic acid C10H12O2[3, 48]

Compound Data



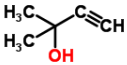
Melting point	**80.00 °C**	**353.15 K**			
CSID	12667	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	1	**ACD/LogP**	2.20
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	O=C(O)C(c1ccccc1)(C)C				
STD InChIKey	YYEROYLAYAVZNW-UHFFFAOYAE				

Melting Points

mp °C	source
81.00	Alfa Aesar
79.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2-methyl-3-butyn-2-ol C5H8O[3, 61, 64]

Compound Data



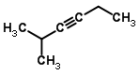
Melting point	**2.87 °C**	**276.02 K**			
CSID	21106133	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	84.1164	**H bond donors**	1	**ACD/LogP**	0.38
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.91 g/cm^3
SMILES	CC(C)(C#C)O				
STD InChIKey	CEBKHWWANWSNTI-UHFFFAOYAU				

Melting Points

mp °C	source
3.00	Alfa Aesar
2.60	Oxford University MSDS
3.00	PHYSPROP

2-methyl-3-hexyne C7H12[4, 64]

Compound Data



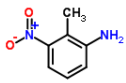
Melting point	**-116.85 °C**	**156.30 K**			
CSID	454272	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.75 g/cm^3
SMILES	C(#CC(C)C)CC				
STD InChIKey	POBOUPFSQKXZFZ-UHFFFAOYAX				

Melting Points

mp °C	source
-117.00	American Petroleum Institute. Research Project 44; Selected ...
-116.70	PHYSPROP

2-methyl-3-nitroaniline C7H8N2O2[3, 64]

Compound Data



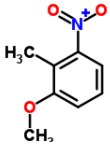
Melting point	**91.00 °C**	**364.15 K**			
CSID	11290	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	2	**ACD/LogP**	1.83
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	[O-][N+](=O)c1cccc(N)c1C				
STD InChIKey	HFCFJYRLBAANKN-UHFFFAOYAO				

Melting Points

mp °C	source

90.00	Alfa Aesar
92.00	PHYSPROP

2-methyl-3-nitroanisole C8H9NO3[3, 64]



Compound Data

Melting point	**54.00 °C**	**327.15 K**			
CSID	70915	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	167.162	**H bond donors**	0	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	[O-][N+](=O)c1cccc(OC)c1C				
STD InChIKey	HQCZLEAGIOIIMC-UHFFFAOYAW				

Melting Points

mp °C	source
53.00	Alfa Aesar
55.00	PHYSPROP

2-methyl-4-nitroaniline C7H8N2O2[3, 64]

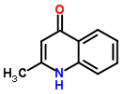
Compound Data

Melting point	**132.75 °C**	**405.90 K**			
CSID	7163	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	2	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	[O-][N+](=O)c1ccc(N)c(c1)C				
STD InChIKey	XTTIQGSLJBWVIV-UHFFFAOYAX				

Melting Points

mp °C	source
132.00	Alfa Aesar
133.50	PHYSPROP

2-methyl-4-quinolinol C10H9NO[3, 64]



Compound Data

Melting point	**234.50 °C**	**507.65 K**			
CSID	62307	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	159.1846	**H bond donors**	1	**ACD/LogP**	3.09
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	O=C\2c1c(cccc1)N/C(=C/2)C				
STD InChIKey	NWINIEGDLHHNLH-UHFFFAOYAE				

Melting Points

mp °C	source
235.00	Alfa Aesar
234.00	PHYSPROP

2-methyl-5-nitroaniline C7H8N2O2[3, 61, 64]

Compound Data

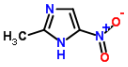
Melting point	**106.67 °C**	**379.82 K**			
CSID	7166	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	2	**ACD/LogP**	1.83
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	[O-][N+](=O)c1cc(N)c(cc1)C				
STD InChIKey	DSBIJCMXAIKKKI-UHFFFAOYAH				

Melting Points

mp °C	source
107.00	Alfa Aesar
107.50	Oxford University MSDS

105.50	PHYSPROP

2-methyl-5-nitroimidazole C4H5N3O2[61, 64, 70]



Compound Data

Melting point	**252.67 °C**	**525.82 K**			
CSID	12236	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	127.1014	**H bond donors**	1	**ACD/LogP**	-0.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	[O-][N+](=O)c1cnc(n1)C				
STD InChIKey	FFYTTYVSDVWNMY-UHFFFAOYAB				

Melting Points

mp °C	source
253.00	Oxford University MSDS
253.00	PHYSPROP
252.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

2-methyl-6-nitroaniline C7H8N2O2[3, 64]

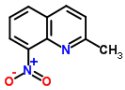
Compound Data

Melting point	**95.50 °C**	**368.65 K**			
CSID	10824	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	2	**ACD/LogP**	2.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	[O-][N+](=O)c1cccc(c1N)C				
STD InChIKey	FCMRHMPITHLLLA-UHFFFAOYAO				

Melting Points

mp °C	source
95.00	Alfa Aesar
96.00	PHYSPROP

2-methyl-8-nitroquinoline C10H8N2O2[3, 64]



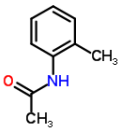
Compound Data

Melting point	**139.00 °C**	**412.15 K**			
CSID	12858	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	188.1827	**H bond donors**	0	**ACD/LogP**	1.93
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	[O-][N+](=O)c1cccc2ccc(nc12)C				
STD InChIKey	UHPGVDHXHDPYQP-UHFFFAOYAN				

Melting Points

mp °C	source
138.00	Alfa Aesar
140.00	PHYSPROP

2-methylacetanilide C9H11NO[3, 64]



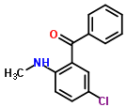
Compound Data

Melting point	**110.50 °C**	**383.65 K**			
CSID	10298354	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	149.1897	**H bond donors**	1	**ACD/LogP**	1.54
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	Cc1ccccc1NC(C)=O				
STD InChIKey	BPEXTIMJLDWDTL-UHFFFAOYAX				

Melting Points

mp °C	source
111.00	Alfa Aesar
110.00	PHYSPROP

2-methylamino-5-chlorobenzophenone C14H12ClNO[3, 61]



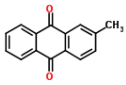
Compound Data

Melting point	**95.00 °C**	**368.15 K**			
CSID	13323	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	245.7042	**H bond donors**	1	**ACD/LogP**	4.66
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	Clc1cc(c(NC)cc1)C(=O)c2ccccc2				
STD InChIKey	WPNMLCMTDCANOZ-UHFFFAOYAQ				

Melting Points

mp °C	source
96.00	Alfa Aesar
94.00	Oxford University MSDS

2-methylanthraquinone C15H10O2[3, 64]



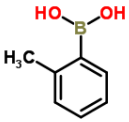
Compound Data

Melting point	**174.50 °C**	**447.65 K**			
CSID	6515	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	222.2387	**H bond donors**	0	**ACD/LogP**	3.84
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	O=C2c1c(cccc1)C(=O)c3c2ccc(c3)C				
STD InChIKey	NJWGQARXZDRHCD-UHFFFAOYAG				

Melting Points

mp °C	source
172.00	Alfa Aesar
177.00	PHYSPROP

2-methylbenzeneboronic acid C7H9BO2[3, 64]



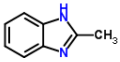
Compound Data

Melting point	**164.75 °C**	**437.90 K**			
CSID	2015070	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.9562	**H bond donors**	2	**ACD/LogP**	2.05
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	OB(O)c1ccccc1C				
STD InChIKey	NSJVYHOPHZMZPN-UHFFFAOYAT				

Melting Points

mp °C	source
163.00	Alfa Aesar
166.50	PHYSPROP

2-methylbenzimidazole C8H8N2[3, 35, 64]



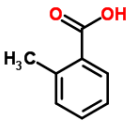
Compound Data

Melting point	**176.33 °C**	**449.48 K**			
CSID	11489	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	132.1625	**H bond donors**	1	**ACD/LogP**	1.57
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	n2c1ccccc1nc2C				
STD InChIKey	LDZYRENCLPUXAX-UHFFFAOYAQ				

Melting Points

mp °C	source
176.00	Alfa Aesar
176.50	EPISuite-ChemSpider
176.50	PHYSPROP

2-methylbenzoic acid C8H8O2[2, 3, 35, 61, 64]



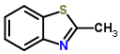
Compound Data

Melting point	**104.48 °C**	**377.63 K**			
CSID	8070	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	1	**ACD/LogP**	2.35
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	O=C(O)c1ccccc1C				
STD InChIKey	ZWLPBLYKEWSWPD-UHFFFAOYAI				

Melting Points

mp °C	source
105.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
105.00	Alfa Aesar
103.70	EPISuite-ChemSpider
105.00	Oxford University MSDS
103.70	PHYSPROP

2-methylbenzothiazole C8H7NS[3, 64]



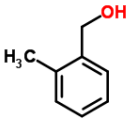
Compound Data

Melting point	**13.00 °C**	**286.15 K**			
CSID	8138	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	149.2129	**H bond donors**	0	**ACD/LogP**	2.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.22 g/cm^3
SMILES	n1c2ccccc2sc1C				
STD InChIKey	DXYYSGDWQCSKKO-UHFFFAOYAE				

Melting Points

mp °C	source
12.00	Alfa Aesar
14.00	PHYSPROP

2-methylbenzyl alcohol C8H10O[2, 3, 64]



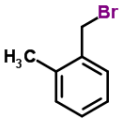
Compound Data

Melting point	**37.33 °C**	**310.48 K**			
CSID	6728	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	1.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.02 g/cm^3
SMILES	OCc1ccccc1C				
STD InChIKey	XPNGNIFUDRPBFJ-UHFFFAOYAO				

Melting Points

mp °C	source
39.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
35.00	Alfa Aesar
38.00	PHYSPROP

2-methylbenzyl bromide C8H9Br[3, 64]



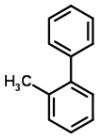
Compound Data

Melting point	**20.00 °C**	**293.15 K**			
CSID	6726	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	185.0611	**H bond donors**	0	**ACD/LogP**	3.38
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	BrCc1ccccc1C				
STD InChIKey	WGVYCXYGPNNUQA-UHFFFAOYAQ				

Melting Points

mp °C	source
19.00	Alfa Aesar
21.00	PHYSPROP

2-methylbiphenyl C13H12[3, 4, 64]



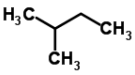
Compound Data

Melting point	**-0.07 °C**	**273.08 K**			
CSID	12044	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	168.2344	**H bond donors**	0	**ACD/LogP**	4.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3
SMILES	c2c(c1ccccc1C)cccc2				
STD InChIKey	ALLIZEAXNXSFGD-UHFFFAOYAX				

Melting Points

mp °C	source
0.00	Alfa Aesar
0.00	American Petroleum Institute. Research Project 44; Selected ...
-0.20	PHYSPROP

2-methylbutane C5H12[4, 61, 64]



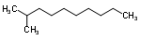
Compound Data

Melting point	**-159.92 °C**	**113.23 K**			
CSID	6308	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	72.1488	**H bond donors**	0	**ACD/LogP**	3.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.65 g/cm^3
SMILES	CC(C)CC				
STD InChIKey	QWTDNUCVQCZILF-UHFFFAOYAE				

Melting Points

mp °C	source
-160.00	American Petroleum Institute. Research Project 44; Selected ...
-160.00	Oxford University MSDS
-159.77	PHYSPROP

2-methyldecane C11H24[4, 64]



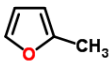
Compound Data

Melting point	**-48.95 °C**	**224.20 K**			
CSID	21896	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	156.3083	**H bond donors**	0	**ACD/LogP**	6.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.74 g/cm^3
SMILES	CCCCCCCCC(C)C				
STD InChIKey	CNPVJWYWYZMPDS-UHFFFAOYAI				

Melting Points

mp °C	source
-49.00	American Petroleum Institute. Research Project 44; Selected ...
-48.90	PHYSPROP

2-methylfuran C5H6O[3, 61, 64]



Compound Data

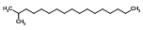
Melting point	**-88.50 °C**	**184.65 K**			
CSID	10340	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	82.1005	**H bond donors**	0	**ACD/LogP**	1.79
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.93 g/cm^3
SMILES	Cc1ccco1				
STD InChIKey	VQKFNUFAXTZWDK-UHFFFAOYAB				

Melting Points

mp °C	source
-89.00	Alfa Aesar
-89.00	Oxford University MSDS

-87.50	PHYSPROP

2-methylheptadecane C18H38[4, 64]



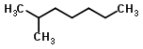
Compound Data

Melting point	**5.85 °C**	**279.00 K**			
CSID	14530	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	254.4943	**H bond donors**	0	**ACD/LogP**	10.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	0.78 g/cm^3
SMILES	C(CCCCCCCC(C)C)CCCCCCC				
STD InChIKey	RJWUMFHQJJBBOD-UHFFFAOYAG				

Melting Points

mp °C	source
6.00	American Petroleum Institute. Research Project 44; Selected ...
5.70	PHYSPROP

2-methylheptane C8H18[4, 64, 64]



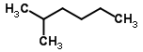
Compound Data

Melting point	**-107.63 °C**	**165.52 K**			
CSID	11106	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.82
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)CCCCC				
STD InChIKey	JVSWJIKNEAIKJW-UHFFFAOYAA				

Melting Points

mp °C	source
-109.00	American Petroleum Institute. Research Project 44; Selected ...
-108.90	PHYSPROP
-105.00	PHYSPROP

2-methylhexane C7H16[4, 64]



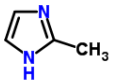
Compound Data

Melting point	**-118.10 °C**	**155.05 K**			
CSID	11094	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.2019	**H bond donors**	0	**ACD/LogP**	4.29
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.69 g/cm^3
SMILES	CC(C)CCCC				
STD InChIKey	GXDHCNNESPLIKD-UHFFFAOYAR				

Melting Points

mp °C	source
-118.00	American Petroleum Institute. Research Project 44; Selected ...
-118.20	PHYSPROP

2-methylimidazole C4H6N2[3, 64]



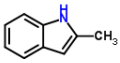
Compound Data

Melting point	**143.50 °C**	**416.65 K**			
CSID	12225	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	82.1038	**H bond donors**	1	**ACD/LogP**	-0.37
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.06 g/cm^3
SMILES	n1ccnc1C				
STD InChIKey	LXBGSDVWAMZHDD-UHFFFAOYAM				

Melting Points

mp °C	source
143.00	Alfa Aesar
144.00	PHYSPROP

2-methylindole C_9H_9N[3, 64]



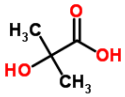
Compound Data

Melting point	**59.50 °C**	**332.65 K**			
CSID	6954	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	131.1745	**H bond donors**	1	**ACD/LogP**	2.60
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c1cccc2c1cc(n2)C				
STD InChIKey	BHNHHSOHWZKFOX-UHFFFAOYAQ				

Melting Points

mp °C	source
58.00	Alfa Aesar
61.00	PHYSPROP

2-methyllactic acid $C_4H_8O_3$[3, 64]



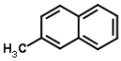
Compound Data

Melting point	**80.75 °C**	**353.90 K**			
CSID	11181	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	104.1045	**H bond donors**	2	**ACD/LogP**	-0.35
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	O=C(O)C(O)(C)C				
STD InChIKey	BWLBGMIXKSTLSX-UHFFFAOYAY				

Melting Points

mp °C	source
79.00	Alfa Aesar
82.50	PHYSPROP

2-methylnaphthalene $C_{11}H_{10}$[3, 64]



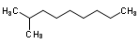
Compound Data

Melting point	**33.70 °C**	**306.85 K**			
CSID	6788	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	142.1971	**H bond donors**	0	**ACD/LogP**	3.91
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.02 g/cm^3
SMILES	c12ccccc1ccc(c2)C				
STD InChIKey	QIMMUPPBPVKWKM-UHFFFAOYAY				

Melting Points

mp °C	source
33.00	Alfa Aesar
34.40	PHYSPROP

2-methylnonane $C_{10}H_{22}$[4, 64]



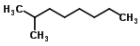
Compound Data

Melting point	**-74.80 °C**	**198.35 K**			
CSID	12807	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.73 g/cm^3
SMILES	CC(CCCCCCC)C				
STD InChIKey	SGVYKUFIHHTIFL-UHFFFAOYAG				

Melting Points

mp °C	source
-75.00	American Petroleum Institute. Research Project 44; Selected ...
-74.60	PHYSPROP

2-methyloctane C_9H_{20}[4, 61, 64]



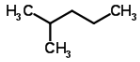
Compound Data

Melting point	**-80.10 °C**	**193.05 K**			
CSID	17558	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	5.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)CCCCCC				
STD InChIKey	ZUBZATZOEPUUQF-UHFFFAOYAO				

Melting Points

mp °C	source
-80.00	American Petroleum Institute. Research Project 44; Selected ...
-80.00	Oxford University MSDS
-80.30	PHYSPROP

2-methylpentane C6H14[3, 4, 61, 64]



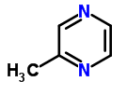
Compound Data

Melting point	**-153.93 °C**	**119.22 K**			
CSID	7604	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	86.1754	**H bond donors**	0	**ACD/LogP**	3.76
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.67 g/cm^3
SMILES	CC(C)CCC				
STD InChIKey	AFABGHUZZDYHJO-UHFFFAOYAZ				

Melting Points

mp °C	source
-154.00	Alfa Aesar
-154.00	American Petroleum Institute. Research Project 44; Selected ...
-154.00	Oxford University MSDS
-153.70	PHYSPROP

2-methylpyrazine C5H6N2[3, 64]



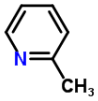
Compound Data

Melting point	**-29.50 °C**	**243.65 K**			
CSID	7688	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.1145	**H bond donors**	0	**ACD/LogP**	0.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.02 g/cm^3
SMILES	n1ccnc(c1)C				
STD InChIKey	CAWHJQAVHZEVTJ-UHFFFAOYAF				

Melting Points

mp °C	source
-30.00	Alfa Aesar
-29.00	PHYSPROP

2-methylpyridine C6H7N[3, 61, 64]



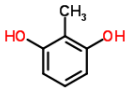
Compound Data

Melting point	**-68.90 °C**	**204.25 K**			
CSID	13839199	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	93.1265	**H bond donors**	0	**ACD/LogP**	1.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.94 g/cm^3
SMILES	Cc1ccccn1				
STD InChIKey	BSKHPKMHTQYZBB-UHFFFAOYAR				

Melting Points

mp °C	source
-70.00	Alfa Aesar
-70.00	Oxford University MSDS
-66.70	PHYSPROP

2-methylresorcinol $C_7H_8O_2$[2, 3, 64]



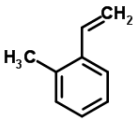
Compound Data

Melting point	**119.33 °C**	**392.48 K**			
CSID	11350	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	1.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	Oc1cccc(O)c1C				
STD InChIKey	ZTMADXFOCUXMJE-UHFFFAOYAE				

Melting Points

mp °C	source
118.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
120.00	Alfa Aesar
120.00	PHYSPROP

2-methylstyrene C_9H_{10}[3, 4, 64]



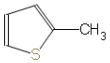
Compound Data

Melting point	**-68.83 °C**	**204.32 K**			
CSID	11410	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.1757	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.90 g/cm^3
SMILES	C=C\c1ccccc1C				
STD InChIKey	NVZWEEGUWXZOKI-UHFFFAOYAK				

Melting Points

mp °C	source
-69.00	Alfa Aesar
-69.00	American Petroleum Institute. Research Project 44; Selected ...
-68.50	PHYSPROP

2-methylthiophene C_5H_6S[3, 64]



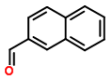
Compound Data

Melting point	**-63.20 °C**	**209.95 K**			
CSID	21168808	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1661	**H bond donors**	0	**ACD/LogP**	2.36
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.03 g/cm^3
SMILES	Cc1cccs1				
STD InChIKey	XQQBUAPQHNYYRS-UHFFFAOYAJ				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-63.40	PHYSPROP

2-naphthaldehyde $C_{11}H_8O$[3, 64]



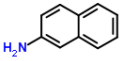
Compound Data

Melting point	**61.50 °C**	**334.65 K**			
CSID	5966	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	156.1806	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	O=Cc2ccc1c(cccc1)c2				
STD InChIKey	PJKVFARRVXDXAD-UHFFFAOYAM				

Melting Points

mp °C	source
61.00	Alfa Aesar
62.00	PHYSPROP

2-naphthalenamine C10H9N[61, 64]



Compound Data

Melting point	**112.25 °C**	**385.40 K**			
CSID	6790	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	2	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	c12ccccc1ccc(N)c2				
STD InChIKey	JBIJLHTVPXGSAM-UHFFFAOYAA				

Melting Points

mp °C	source
111.50	Oxford University MSDS
113.00	PHYSPROP

2-naphthalenamine C6H7N3O2[61, 64]

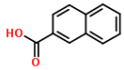
Compound Data

Melting point	**139.25 °C**	**412.40 K**			
CSID	3542441	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	153.1387	**H bond donors**	4	**ACD/LogP**	0.91
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.45 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1N)N				
STD InChIKey	HVHNMNGARPCGGD-UHFFFAOYAX				

Melting Points

mp °C	source
138.50	Oxford University MSDS
140.00	PHYSPROP

2-naphthoic acid C11H8O2[3, 64]



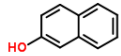
Compound Data

Melting point	**184.75 °C**	**457.90 K**			
CSID	6856	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.18	**H bond donors**	1	**ACD/LogP**	3.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	O=C(O)c2ccc1c(cccc1)c2				
STD InChIKey	UOBYKYZJUGYBDK-UHFFFAOYAM				

Melting Points

mp °C	source
184.00	Alfa Aesar
185.50	PHYSPROP

2-naphthol C10H8O[2, 3, 44, 61, 64]



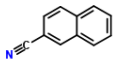
Compound Data

Melting point	**122.40 °C**	**395.55 K**			
CSID	8341	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	144.1699	**H bond donors**	1	**ACD/LogP**	2.72
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	c1ccc2cc(ccc2c1)O				
STD InChIKey	JWAZRIHNYRIHIV-UHFFFAOYAV				

Melting Points

mp °C	source
123.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
122.00	Alfa Aesar
122.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
122.00	Oxford University MSDS
123.00	PHYSPROP

2-naphthonitrile C11H7N[3, 64]



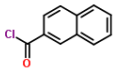
Compound Data

Melting point	**65.50 °C**	**338.65 K**			
CSID	11450	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	153.18	**H bond donors**	0	**ACD/LogP**	2.89
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	N#Cc2ccc1c(cccc1)c2				
STD InChIKey	AZKDTTQQTKDXLH-UHFFFAOYAM				

Melting Points

mp °C	source
65.00	Alfa Aesar
66.00	PHYSPROP

2-naphthoyl chloride C11H7ClO[3, 64]



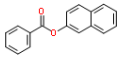
Compound Data

Melting point	**50.50 °C**	**323.65 K**			
CSID	67790	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	190.6257	**H bond donors**	0	**ACD/LogP**	3.44
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	ClC(=O)c2ccc1c(cccc1)c2				
STD InChIKey	XNLBCXGRQWUJLU-UHFFFAOYAX				

Melting Points

mp °C	source
50.00	Alfa Aesar
51.00	PHYSPROP

2-naphthyl benzoate C17H12O2[3, 48, 64]



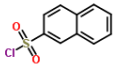
Compound Data

Melting point	**106.33 °C**	**379.48 K**			
CSID	60100	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	248.276	**H bond donors**	0	**ACD/LogP**	4.82
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.20 g/cm^3
SMILES	O=C(Oc2ccc1c(cccc1)c2)c3ccccc3				
STD InChIKey	DWJIJRSTYFPKGD-UHFFFAOYAH				

Melting Points

mp °C	source
107.00	Alfa Aesar
105.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
107.00	PHYSPROP

2-naphthylsulfonyl chloride C10H7ClO2S[3, 64]



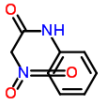
Compound Data

Melting point	**78.50 °C**	**351.65 K**			
CSID	6858	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	226.6794	**H bond donors**	0	**ACD/LogP**	3.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.41 g/cm^3
SMILES	ClS(=O)(=O)c2ccc1c(cccc1)c2				
STD InChIKey	OPECTNGATDYLSS-UHFFFAOYAP				

Melting Points

mp °C	source
76.00	Alfa Aesar
81.00	PHYSPROP

2-nitro-N-phenylacetamide C8H8N2O3[61, 64]



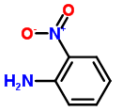
Compound Data

Melting point	**93.50 °C**	**366.65 K**			
CSID	11279086	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	180.1607	**H bond donors**	1	**ACD/LogP**	1.25
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.33 g/cm^3
SMILES	O=C(Nc1ccccc1)CN(=O)=O				
STD InChIKey	JFPJVTNYCURRAB-UHFFFAOYAL				

Melting Points

mp °C	source
93.00	Oxford University MSDS
94.00	PHYSPROP

2-nitroaniline C6H6N2O2[2, 3, 61, 64]



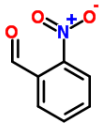
Compound Data

Melting point	**72.00 °C**	**345.15 K**			
CSID	13853943	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	138.124	**H bond donors**	2	**ACD/LogP**	1.83
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1N				
STD InChIKey	DPJCXCZTLWNFOH-UHFFFAOYAV				

Melting Points

mp °C	source
73.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
72.00	Alfa Aesar
72.00	Oxford University MSDS
71.00	PHYSPROP

2-nitrobenzaldehyde C7H5NO3[2, 3, 64]



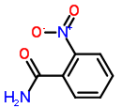
Compound Data

Melting point	**44.83 °C**	**317.98 K**			
CSID	10630	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	151.1195	**H bond donors**	0	**ACD/LogP**	1.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1C=O				
STD InChIKey	CMWKITSNTDAEDT-UHFFFAOYAD				

Melting Points

mp °C	source
46.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
45.00	Alfa Aesar
43.50	PHYSPROP

2-nitrobenzamide C7H6N2O3[3, 7, 64]



Compound Data

Melting point	**176.20 °C**	**449.35 K**			
CSID	11178542	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	166.1341	**H bond donors**	2	**ACD/LogP**	0.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1C(N)=O				
STD InChIKey	KLGQWSOYKYFBTR-UHFFFAOYAM				

Melting Points

mp °C	source
176.00	Alfa Aesar
176.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
176.60	PHYSPROP

2-nitrobenzhydrazide C7H7N3O3[3, 64]

Compound Data

Melting point	**122.50 °C**	**395.65 K**			
CSID	3009396	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	181.1488	**H bond donors**	3	**ACD/LogP**	-0.54
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.41 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1C(=O)NN				
STD InChIKey	LYGGDXLOJMNFBV-UHFFFAOYAW				

Melting Points

mp °C	source
121.00	Alfa Aesar
124.00	PHYSPROP

2-nitrobenzoic acid C7H5NO4[2, 3, 61, 64]

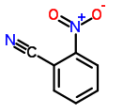
Compound Data

Melting point	**147.62 °C**	**420.77 K**			
CSID	10616	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	167.1189	**H bond donors**	1	**ACD/LogP**	1.19
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	c1ccc(c(c1)C(=O)O)[N+](=O)[O-]				
STD InChIKey	SLAMLWHELXOEJZ-UHFFFAOYAQ				

Melting Points

mp °C	source
148.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
148.00	Alfa Aesar
147.00	Oxford University MSDS
147.50	PHYSPROP

2-nitrobenzonitrile C7H4N2O2[2, 3, 64]



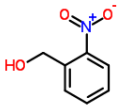
Compound Data

Melting point	**108.67 °C**	**381.82 K**			
CSID	11428	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	148.1189	**H bond donors**	0	**ACD/LogP**	1.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.31 g/cm^3
SMILES	N#Cc1ccccc1[N+]([O-])=O				
STD InChIKey	SWBDKCMOLSUXRH-UHFFFAOYAB				

Melting Points

mp °C	source
109.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
109.00	Alfa Aesar
108.00	PHYSPROP

2-nitrobenzyl alcohol C7H7NO3[2, 3, 64]



Compound Data

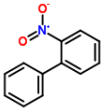
Melting point	**72.67 °C**	**345.82 K**			
CSID	11429	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	153.1354	**H bond donors**	1	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.33 g/cm^3
SMILES	[O-][N+](=O)c1ccccc1CO				
STD InChIKey	BWRBVBFLFQKBPT-UHFFFAOYAQ				

Melting Points

mp °C	source
72.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

72.00	Alfa Aesar
74.00	PHYSPROP

2-nitrobiphenyl C12H9NO2[7, 64]



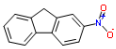
Compound Data

Melting point	**37.10 °C**	**310.25 K**			
CSID	21106576	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	199.2054	**H bond donors**	0	**ACD/LogP**	3.52
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	[O-][N+](=O)c2ccccc2c1ccccc1				
STD InChIKey	YOJKKXRJMXIKSR-UHFFFAOYAD				

Melting Points

mp °C	source
37.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
37.20	PHYSPROP

2-nitrofluorene C13H9NO2[61, 64]



Compound Data

Melting point	**156.50 °C**	**429.65 K**			
CSID	11338	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	211.2161	**H bond donors**	0	**ACD/LogP**	3.89
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	[O-][N+](=O)c3ccc2c1ccccc1Cc2c3				
STD InChIKey	XFOHWECQTFIEIX-UHFFFAOYAJ				

Melting Points

mp °C	source
156.00	Oxford University MSDS
157.00	PHYSPROP

2-nitrofuran C4H3NO3[61, 64]

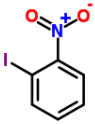
Compound Data

Melting point	**30.50 °C**	**303.65 K**			
CSID	11372	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	113.0715	**H bond donors**	0	**ACD/LogP**	0.78
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	[O-][N+](=O)c1occc1				
STD InChIKey	FUBFWTUFPGFHOJ-UHFFFAOYAQ				

Melting Points

mp °C	source
31.00	Oxford University MSDS
30.00	PHYSPROP

2-nitroiodobenzene C6H4INO2[2, 3, 61, 64]



Compound Data

Melting point	**51.25 °C**	**324.40 K**			
CSID	62332	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	249.0059	**H bond donors**	0	**ACD/LogP**	2.76
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.02 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1I				
STD InChIKey	JXMZUNPWVXQADG-UHFFFAOYAZ				

Melting Points

mp °C	source
51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
50.00	Alfa Aesar

50.00	Oxford University MSDS
54.00	PHYSPROP

2-nitrophenol C6H5NO3[3, 7, 28, 48, 56, 61, 64, 72]

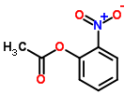
Compound Data

Melting point	**44.76 °C**	**317.91 K**			
CSID	13837787	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	139.1088	**H bond donors**	1	**ACD/LogP**	1.71
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.40 g/cm^3
SMILES	O=N(=O)c1ccccc1O				
STD InChIKey	IQUPABOKLQSFBK-UHFFFAOYAO				

Melting Points

mp °C	source
46.00	Alfa Aesar
45.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
44.80	CRC Handbook of Chemistry and Physics
45.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
44.50	Merck Index
44.00	Oxford University MSDS
44.80	PHYSPROP
44.00	Sigma-Aldrich

2-nitrophenyl acetate C8H7NO4[2, 64]



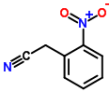
Compound Data

Melting point	**40.25 °C**	**313.40 K**			
CSID	11397	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	181.1455	**H bond donors**	0	**ACD/LogP**	1.55
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.30 g/cm^3
SMILES	O=C(Oc1ccccc1[N+]([O-])=O)C				
STD InChIKey	MRCKRGSNLOHYRA-UHFFFAOYAR				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
40.50	PHYSPROP

2-nitrophenylacetonitrile C8H6N2O2[2, 3, 48, 61, 64]



Compound Data

Melting point	**83.40 °C**	**356.55 K**			
CSID	11395	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	162.1454	**H bond donors**	0	**ACD/LogP**	1.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	N#CCc1ccccc1[N+]([O-])=O				
STD InChIKey	YPRFCQAWSNWRLM-UHFFFAOYAZ				

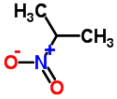
Melting Points

mp °C	source
84.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
83.00	Alfa Aesar
82.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
84.00	Oxford University MSDS
84.00	PHYSPROP

2-nitropropane C3H7NO2[2, 61, 64]

Compound Data

Melting point	**-92.43 °C**	**180.72 K**			
CSID	387	**H bond acceptors**	3	**Rule of 5 violations**	0



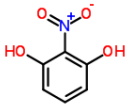
Molecular weight	89.09	**H bond donors**	0	**ACD/LogP**	0.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3
SMILES	CC(C)[N+](=O)[O-]				
STD InChIKey	FGLBSLMDCBOPQK-UHFFFAOYAM				

Melting Points

mp °C	source
-93.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-93.00	Oxford University MSDS
-91.30	PHYSPROP

2-nitroresorcinol C6H5NO4[3, 64]

Compound Data



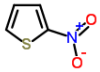
Melting point	**82.50 °C**	**355.65 K**			
CSID	11267	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	155.1082	**H bond donors**	2	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.58 g/cm^3
SMILES	O=[N+]([O-])c1c(O)cccc1O				
STD InChIKey	ZLCPKMIJYMHZMJ-UHFFFAOYAG				

Melting Points

mp °C	source
83.00	Alfa Aesar
82.00	PHYSPROP

2-nitrothiophene C4H3NO2S[3, 64]

Compound Data



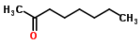
Melting point	**45.25 °C**	**318.40 K**			
CSID	11373	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	129.1371	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.42 g/cm^3
SMILES	[O-][N+](=O)c1sccc1				
STD InChIKey	JIZRGGUCOQKGQD-UHFFFAOYAL				

Melting Points

mp °C	source
44.00	Alfa Aesar
46.50	PHYSPROP

2-octanone C8H16O[3, 4, 64]

Compound Data



Melting point	**-17.67 °C**	**255.48 K**			
CSID	7802	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	128.212	**H bond donors**	0	**ACD/LogP**	2.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.81 g/cm^3
SMILES	O=C(C)CCCCCC				
STD InChIKey	ZPVFWPFBNIEHGJ-UHFFFAOYAR				

Melting Points

mp °C	source
-16.00	Alfa Aesar
-21.00	American Petroleum Institute. Research Project 44; Selected ...
-16.00	PHYSPROP

2-oxetanone C3H4O2[3, 64]

Compound Data

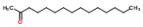
Melting point	**-33.70 °C**	**239.45 K**			
CSID	2275	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	72.0627	**H bond donors**	0	**ACD/LogP**	-1.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3
SMILES	O=C1OCC1				
STD InChIKey	VEZXCJBBBCKRPI-UHFFFAOYAQ				

Melting Points

mp °C	source
-34.00	Alfa Aesar
-33.40	PHYSPROP

2-pentadecanone C15H30O[3, 64]

Compound Data



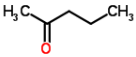
Melting point	**39.25 °C**	**312.40 K**			
CSID	55242	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	226.3981	**H bond donors**	0	**ACD/LogP**	6.22
Phase 25 °C	solid	**Rotatable bonds**	12	**Predicted density**	0.83 g/cm^3
SMILES	CC(=O)CCCCCCCCCCCCC				
STD InChIKey	CJPNOLIZCWDHJK-UHFFFAOYAR				

Melting Points

mp °C	source
39.00	Alfa Aesar
39.50	PHYSPROP

2-pentanone C5H10O[3, 4, 61, 64]

Compound Data



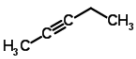
Melting point	**-77.72 °C**	**195.42 K**			
CSID	7607	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	86.1323	**H bond donors**	0	**ACD/LogP**	0.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.80 g/cm^3
SMILES	O=C(C)CCC				
STD InChIKey	XNLICIUVMPYHGG-UHFFFAOYAJ				

Melting Points

mp °C	source
-78.00	Alfa Aesar
-78.00	American Petroleum Institute. Research Project 44; Selected ...
-78.00	Oxford University MSDS
-76.90	PHYSPROP

2-pentyne C5H8[3, 4, 64]

Compound Data

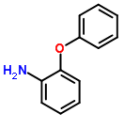


Melting point	**-109.10 °C**	**164.05 K**			
CSID	11807	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	68.117	**H bond donors**	0	**ACD/LogP**	1.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.72 g/cm^3
SMILES	C(#CCC)C				
STD InChIKey	NKTDTMONXHODTI-UHFFFAOYAI				

Melting Points

mp °C	source
-109.00	Alfa Aesar
-109.00	American Petroleum Institute. Research Project 44; Selected ...
-109.30	PHYSPROP

2-phenoxyaniline C12H11NO[3, 64]



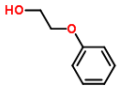
Compound Data

Melting point	**46.40 °C**	**319.55 K**			
CSID	68404	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	185.2218	**H bond donors**	2	**ACD/LogP**	2.46
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	O(c1ccccc1)c2ccccc2N				
STD InChIKey	NMFFUUFPJJOWHK-UHFFFAOYAR				

Melting Points

mp °C	source
47.00	Alfa Aesar
45.80	PHYSPROP

2-phenoxyethanol C8H10O2[2, 3, 61, 64]



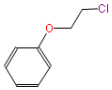
Compound Data

Melting point	**12.75 °C**	**285.90 K**			
CSID	13848467	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	1	**ACD/LogP**	1.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.08 g/cm^3
SMILES	c1ccc(cc1)OCCO				
STD InChIKey	QCDWFXQBSFUVSP-UHFFFAOYAU				

Melting Points

mp °C	source
13.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
12.00	Alfa Aesar
12.00	Oxford University MSDS
14.00	PHYSPROP

2-phenoxyethyl chloride C8H9ClO[3, 7, 64]



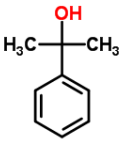
Compound Data

Melting point	**26.67 °C**	**299.82 K**			
CSID	21168833	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	156.6095	**H bond donors**	0	**ACD/LogP**	2.59
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	ClCCOc1ccccc1				
STD InChIKey	VQUYNUJARXBNPK-UHFFFAOYAV				

Melting Points

mp °C	source
24.00	Alfa Aesar
28.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
28.00	PHYSPROP

2-phenyl-2-propanol C9H12O[2, 3, 64]



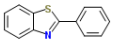
Compound Data

Melting point	**34.00 °C**	**307.15 K**			
CSID	11556	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	1	**ACD/LogP**	1.73
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	OC(c1ccccc1)(C)C				
STD InChIKey	BDCFWIDZNLCTMF-UHFFFAOYAG				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar
36.00	PHYSPROP

2-phenylbenzothiazole C13H9NS[3, 64]



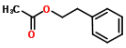
Compound Data

Melting point	**114.50 °C**	**387.65 K**			
CSID	12864	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	211.2823	**H bond donors**	0	**ACD/LogP**	4.26
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	n1c3ccccc3sc1c2ccccc2				
STD InChIKey	XBHOUXSGHYZCNH-UHFFFAOYAN				

Melting Points

mp °C	source
114.00	Alfa Aesar
115.00	PHYSPROP

2-phenylethyl acetate C10H12O2[3, 64]



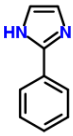
Compound Data

Melting point	**-31.05 °C**	**242.10 K**			
CSID	21105987	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	0	**ACD/LogP**	2.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.03 g/cm^3
SMILES	CC(=O)OCCc1ccccc1				
STD InChIKey	MDHYEMXUFSJLGV-UHFFFAOYAK				

Melting Points

mp °C	source
-31.00	Alfa Aesar
-31.10	PHYSPROP

2-phenylimidazole C9H8N2[3, 64]



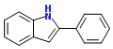
Compound Data

Melting point	**148.65 °C**	**421.80 K**			
CSID	62795	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.1732	**H bond donors**	1	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	n1ccnc1c2ccccc2				
STD InChIKey	ZCUJYXPAKHMBAZ-UHFFFAOYAE				

Melting Points

mp °C	source
148.00	Alfa Aesar
149.30	PHYSPROP

2-phenylindole C14H11N[3, 64]



Compound Data

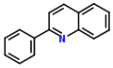
Melting point	**190.25 °C**	**463.40 K**			
CSID	13105	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	193.2438	**H bond donors**	1	**ACD/LogP**	4.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	c1cccc3c1cc(c2ccccc2)n3				
STD InChIKey	KLLLJCACIRKBDT-UHFFFAOYAH				

Melting Points

mp °C	source
190.00	Alfa Aesar
190.50	PHYSPROP

2-phenylquinoline C15H11N[3, 64]

Compound Data



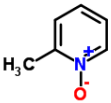
Melting point	**84.50 °C**	**357.65 K**			
CSID	64618	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	205.2545	**H bond donors**	0	**ACD/LogP**	4.19
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	c1ccc(cc1)c2ccc3ccccc3n2				
STD InChIKey	FSEXLNMNADBYJU-UHFFFAOYAP				

Melting Points

mp °C	source
83.00	Alfa Aesar
86.00	PHYSPROP

2-picoline N-oxide C6H7NO[3, 64]

Compound Data



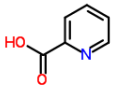
Melting point	**48.50 °C**	**321.65 K**			
CSID	13013	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	0	**ACD/LogP**	-0.74
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.01 g/cm^3
SMILES	[O-][n+]1ccccc1C				
STD InChIKey	CFZKDDTWZYUZKS-UHFFFAOYAG				

Melting Points

mp °C	source
48.00	Alfa Aesar
49.00	PHYSPROP

2-picolinic acid C6H5NO2[3, 64]

Compound Data



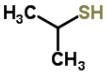
Melting point	**136.75 °C**	**409.90 K**			
CSID	993	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	123.1094	**H bond donors**	1	**ACD/LogP**	0.24
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	c1ccnc(c1)C(=O)O				
STD InChIKey	SIOXPEMLGUPBBT-UHFFFAOYAC				

Melting Points

mp °C	source
137.00	Alfa Aesar
136.50	PHYSPROP

2-propanethiol C3H8S[3, 4, 64]

Compound Data



Melting point	**-130.83 °C**	**142.32 K**			
CSID	6124	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	76.1606	**H bond donors**	0	**ACD/LogP**	1.59
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.82 g/cm^3
SMILES	SC(C)C				
STD InChIKey	KJRCEJOSASVSRA-UHFFFAOYAY				

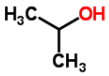
Melting Points

mp °C	source
-131.00	Alfa Aesar
-131.00	American Petroleum Institute. Research Project 44; Selected ...
-130.50	PHYSPROP

2-propanol C3H8O[3, 4, 32, 64]

Compound Data

Melting point	**-89.25 °C**	**183.90 K**



CSID	3644	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	60.095	**H bond donors**	1	**ACD/LogP**	0.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.79 g/cm^3
SMILES	CC(C)O				
STD InChIKey	KFZMGEQAYNKOFK-UHFFFAOYAH				

Melting Points

mp °C	source
-90.00	Alfa Aesar
-88.00	American Petroleum Institute. Research Project 44; Selected ...
-89.50	DrugBank
-89.50	PHYSPROP

2-pyridinethiol C5H5NS[3, 61, 64]

Compound Data

Melting point	**128.33 °C**	**401.48 K**			
CSID	2005897	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	111.1649	**H bond donors**	1	**ACD/LogP**	0.32
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	S=C1/C=C\C=C/N1				
STD InChIKey	WHMDPDGBKYUEMW-UHFFFAOYAE				

Melting Points

mp °C	source
127.00	Alfa Aesar
129.00	Oxford University MSDS
129.00	PHYSPROP

2-pyrrolidinone C4H7NO[3, 64]

Compound Data

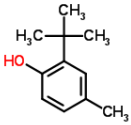
Melting point	**23.50 °C**	**296.65 K**			
CSID	11530	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	85.1045	**H bond donors**	1	**ACD/LogP**	-1.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	O=C1NCCC1				
STD InChIKey	HNJBEVLQSNELDL-UHFFFAOYAP				

Melting Points

mp °C	source
24.00	Alfa Aesar
23.00	PHYSPROP

2-t-butyl-4-methylphenol C11H16O[3, 64]

Compound Data

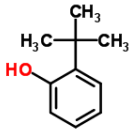


Melting point	**51.75 °C**	**324.90 K**			
CSID	16109	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	164.2441	**H bond donors**	1	**ACD/LogP**	3.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.96 g/cm^3
SMILES	Oc1ccc(cc1C(C)(C)C)C				
STD InChIKey	IKEHOXWJQXIQAG-UHFFFAOYAH				

Melting Points

mp °C	source
52.00	Alfa Aesar
51.50	PHYSPROP

2-t-butylphenol C10H14O[3, 64]



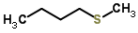
Compound Data

Melting point	**-6.90 °C**	**266.25 K**			
CSID	6657	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	1	**ACD/LogP**	3.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	Oc1ccccc1C(C)(C)C				
STD InChIKey	WJQOZHYUIDYNHM-UHFFFAOYAN				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-6.80	PHYSPROP

2-thiahexane C5H12S[4, 64]



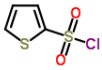
Compound Data

Melting point	**-97.90 °C**	**175.25 K**			
CSID	11834	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	104.2138	**H bond donors**	0	**ACD/LogP**	2.48
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.83 g/cm^3
SMILES	S(CCCC)C				
STD InChIKey	WCXXISMIJBRDQK-UHFFFAOYAX				

Melting Points

mp °C	source
-98.00	American Petroleum Institute. Research Project 44; Selected ...
-97.80	PHYSPROP

2-thienylsulfonyl chloride C4H3ClO2S2[3, 64]



Compound Data

Melting point	**29.00 °C**	**302.15 K**			
CSID	77127	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	182.6484	**H bond donors**	0	**ACD/LogP**	1.67
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.58 g/cm^3
SMILES	ClS(=O)(=O)c1sccc1				
STD InChIKey	VNNLHYZDXIBHKZ-UHFFFAOYAM				

Melting Points

mp °C	source
30.00	Alfa Aesar
28.00	PHYSPROP

2-toluenesulfonamide C7H9NO2S[3, 64]

Compound Data

Melting point	**156.15 °C**	**429.30 K**			
CSID	6658	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.2169	**H bond donors**	2	**ACD/LogP**	0.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	O=S(=O)(c1ccccc1C)N				
STD InChIKey	YCMLQMDWSXFTIF-UHFFFAOYAB				

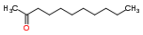
Melting Points

mp °C	source
156.00	Alfa Aesar
156.30	PHYSPROP

2-undecanone C11H22O[3, 4, 61, 64]

Compound Data

Melting point	**13.00 °C**	**286.15 K**	



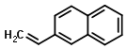
CSID	7871	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2918	**H bond donors**	0	**ACD/LogP**	4.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.82 g/cm^3
SMILES	O=C(CCCCCCCCC)C				
STD InChIKey	KYWIYKKSMDLRDC-UHFFFAOYAV				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.00	American Petroleum Institute. Research Project 44; Selected ...
12.00	Oxford University MSDS
15.00	PHYSPROP

2-vinylnaphthalene C12H10[3, 64]

Compound Data



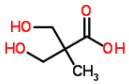
Melting point	**65.50 °C**	**338.65 K**			
CSID	12675	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	154.2078	**H bond donors**	0	**ACD/LogP**	3.93
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.03 g/cm^3
SMILES	c12ccccc1ccc(\C=C)c2				
STD InChIKey	KXYAVSFOJVUIHT-UHFFFAOYAO				

Melting Points

mp °C	source
65.00	Alfa Aesar
66.00	PHYSPROP

2,2-bis(hydroxymethyl)propionic acid C5H10O4[3, 64]

Compound Data



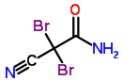
Melting point	**189.50 °C**	**462.65 K**			
CSID	70865	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	134.1305	**H bond donors**	3	**ACD/LogP**	-1.90
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.33 g/cm^3
SMILES	O=C(O)C(C)(CO)CO				
STD InChIKey	PTBDIHRZYDMNKB-UHFFFAOYAV				

Melting Points

mp °C	source
189.00	Alfa Aesar
190.00	PHYSPROP

2,2-dibromo-2-cyanoacetamide C3H2Br2N2O[61, 64]

Compound Data



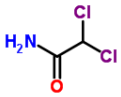
Melting point	**124.00 °C**	**397.15 K**			
CSID	23422	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	241.8688	**H bond donors**	2	**ACD/LogP**	1.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.45 g/cm^3
SMILES	BrC(Br)(C#N)C(=O)N				
STD InChIKey	UUIVKBHZENILKB-UHFFFAOYAS				

Melting Points

mp °C	source
123.50	Oxford University MSDS
124.50	PHYSPROP

2,2-dichloroacetamide C2H3Cl2NO[3, 64]

Compound Data



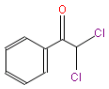
Melting point	**99.20 °C**	**372.35 K**			
CSID	12173	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	127.9573	**H bond donors**	2	**ACD/LogP**	-0.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.50 g/cm^3
SMILES	ClC(Cl)C(=O)N				
STD InChIKey	WCGGWVOVFQNRRS-UHFFFAOYAX				

Melting Points

mp °C	source
99.00	Alfa Aesar
99.40	PHYSPROP

2,2-dichloroacetophenone C8H6Cl2O[3, 64]

Compound Data



Melting point	**20.75 °C**	**293.90 K**			
CSID	21169500	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	189.0386	**H bond donors**	0	**ACD/LogP**	2.38
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=C(C(Cl)Cl)c1ccccc1				
STD InChIKey	CERJZAHSUZVMCH-UHFFFAOYAC				

Melting Points

mp °C	source
21.00	Alfa Aesar
20.50	PHYSPROP

2,2-dichloropropane C3H6Cl2[31, 64]

Compound Data

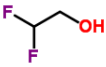
Melting point	**-33.90 °C**	**239.25 K**			
CSID	11170	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.9857	**H bond donors**	0	**ACD/LogP**	1.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.12 g/cm^3
SMILES	ClC(Cl)(C)C				
STD InChIKey	ZEOVXNVKXIPWMS-UHFFFAOYAS				

Melting Points

mp °C	source
-34.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-33.80	PHYSPROP

2,2-difluoroethanol C2H4F2O[3, 64]

Compound Data



Melting point	**-28.10 °C**	**245.05 K**			
CSID	119963	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	82.0494	**H bond donors**	1	**ACD/LogP**	-0.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	FC(F)CO				
STD InChIKey	VOGSDFLJZPNWHY-UHFFFAOYAM				

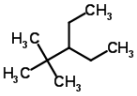
Melting Points

mp °C	source
-28.00	Alfa Aesar
-28.20	PHYSPROP

2,2-dimethyl-3-ethylpentane C9H20[4, 64]

Compound Data

Melting point	**-99.15 °C**	**174.00 K**			
CSID	26068	**H bond acceptors**	0	**Rule of 5 violations**	0



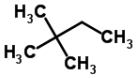
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.72 g/cm^3
SMILES	CCC(CC)C(C)(C)C				
STD InChIKey	CLZCPQKGOAXOJT-UHFFFAOYAN				

Melting Points

mp °C	source
-99.00	American Petroleum Institute. Research Project 44; Selected ...
-99.30	PHYSPROP

2,2-dimethylbutane C6H14[3, 4, 61, 64]

Compound Data



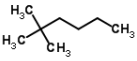
Melting point	**-99.75 °C**	**173.40 K**			
CSID	6163	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	86.1754	**H bond donors**	0	**ACD/LogP**	3.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.68 g/cm^3
SMILES	CC(C)(C)CC				
STD InChIKey	HNRMPXKDFBEGFZ-UHFFFAOYAJ				

Melting Points

mp °C	source
-100.00	Alfa Aesar
-100.00	American Petroleum Institute. Research Project 44; Selected ...
-100.00	Oxford University MSDS
-99.00	PHYSPROP

2,2-dimethylhexane C8H18[4, 64]

Compound Data



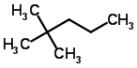
Melting point	**-121.05 °C**	**152.10 K**			
CSID	11064	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.64
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)(C)CCCC				
STD InChIKey	FLTJDUOFAQWHDF-UHFFFAOYAU				

Melting Points

mp °C	source
-121.00	American Petroleum Institute. Research Project 44; Selected ...
-121.10	PHYSPROP

2,2-dimethylpentane C7H16[4, 64]

Compound Data



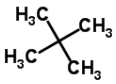
Melting point	**-123.90 °C**	**149.25 K**			
CSID	11055	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.2019	**H bond donors**	0	**ACD/LogP**	4.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.69 g/cm^3
SMILES	CC(C)(C)CCC				
STD InChIKey	CXOWYJMDMMMMJO-UHFFFAOYAN				

Melting Points

mp °C	source
-124.00	American Petroleum Institute. Research Project 44; Selected ...
-123.80	PHYSPROP

2,2-dimethylpropane C5H12[4, 64]

Compound Data



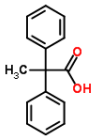
Melting point	**-16.70 °C**	**256.45 K**			
CSID	9646	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	72.1488	**H bond donors**	0	**ACD/LogP**	3.05
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.65 g/cm^3
SMILES	CC(C)(C)C				
STD InChIKey	CRSOQBOWXPBRES-UHFFFAOYAR				

Melting Points

mp °C	source
-17.00	American Petroleum Institute. Research Project 44; Selected ...
-16.40	PHYSPROP

2,2-diphenylpropionic acid C15H14O2[48, 64]

Compound Data



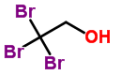
Melting point	**174.50 °C**	**447.65 K**			
CSID	71976	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	226.2705	**H bond donors**	1	**ACD/LogP**	3.60
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	O=C(O)C(c1ccccc1)(c2ccccc2)C				
STD InChIKey	ODELFXJUOVNEFZ-UHFFFAOYAO				

Melting Points

mp °C	source
173.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
176.00	PHYSPROP

2,2,2-tribromoethanol C2H3Br3O[3, 64]

Compound Data



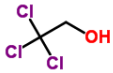
Melting point	**80.00 °C**	**353.15 K**			
CSID	6160	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	282.7566	**H bond donors**	1	**ACD/LogP**	2.30
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.87 g/cm^3
SMILES	BrC(Br)(Br)CO				
STD InChIKey	YFDSDPIBEUFTMI-UHFFFAOYAI				

Melting Points

mp °C	source
79.00	Alfa Aesar
81.00	PHYSPROP

2,2,2-trichloroethanol C2H3Cl3O[3, 64]

Compound Data



Melting point	**18.50 °C**	**291.65 K**			
CSID	7961	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	149.4036	**H bond donors**	1	**ACD/LogP**	1.38
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.60 g/cm^3
SMILES	ClC(Cl)(Cl)CO				
STD InChIKey	KPWDGTGXUYRARH-UHFFFAOYAW				

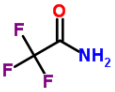
Melting Points

mp °C	source
18.00	Alfa Aesar
19.00	PHYSPROP

2,2,2-trifluoroacetamide C2H2F3NO[3, 64]

Compound Data

Melting point	**72.75 °C**	**345.90 K**			
CSID	61036	**H bond acceptors**	2	**Rule of 5 violations**	0



Molecular weight	113.0386	**H bond donors**	2	**ACD/LogP**	0.17
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.44 g/cm^3
SMILES	FC(F)(F)C(=O)N				
STD InChIKey	NRKYWOKHZRQRJR-UHFFFAOYAD				

Melting Points

mp °C	source
73.00	Alfa Aesar
72.50	PHYSPROP

2,2,2-trifluoroethanol C2H3F3O[3, 61, 64]

Compound Data

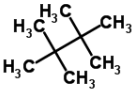
Melting point	**-43.67 °C**	**229.48 K**			
CSID	21106169	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	100.0398	**H bond donors**	1	**ACD/LogP**	0.31
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	FC(F)(F)CO				
STD InChIKey	RHQDFWAXVIIEBN-UHFFFAOYAH				

Melting Points

mp °C	source
-44.00	Alfa Aesar
-43.50	Oxford University MSDS
-43.50	PHYSPROP

2,2,3,3-tetramethylbutane C8H18[4, 64]

Compound Data



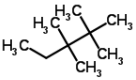
Melting point	**100.85 °C**	**374.00 K**			
CSID	11185	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)(C)C(C)(C)C				
STD InChIKey	OMMLUKLXGSRPHK-UHFFFAOYAD				

Melting Points

mp °C	source
101.00	American Petroleum Institute. Research Project 44; Selected ...
100.70	PHYSPROP

2,2,3,3-tetramethylpentane C9H20[4, 64]

Compound Data



Melting point	**-9.90 °C**	**263.25 K**			
CSID	83703	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)(C)C(C)(C)CC				
STD InChIKey	QUKOJKFJIHSBKV-UHFFFAOYAN				

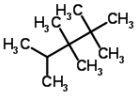
Melting Points

mp °C	source
-10.00	American Petroleum Institute. Research Project 44; Selected ...
-9.80	PHYSPROP

2,2,3,3,4-pentamethylpentane C10H22[4, 64]

Compound Data

Melting point	**-36.20 °C**	**236.95 K**



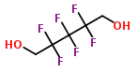
CSID	452968	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.73 g/cm^3
SMILES	CC(C)(C)C(C)(C)C(C)C				
STD InChIKey	WKQBIIUOSATALN-UHFFFAOYAR				

Melting Points

mp °C	source
-36.00	American Petroleum Institute. Research Project 44; Selected ...
-36.40	PHYSPROP

2,2,3,3,4,4-hexafluoro-1,5-pentanediol C5H6F6O2[3, 64]

Compound Data



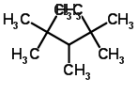
Melting point	**78.75 °C**	**351.90 K**			
CSID	61148	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.0904	**H bond donors**	2	**ACD/LogP**	0.92
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.53 g/cm^3
SMILES	FC(F)(C(F)(F)CO)C(F)(F)CO				
STD InChIKey	IELVMUPSWDZWSD-UHFFFAOYAZ				

Melting Points

mp °C	source
78.00	Alfa Aesar
79.50	PHYSPROP

2,2,3,4,4-pentamethylpentane C10H22[4, 64]

Compound Data



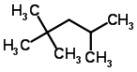
Melting point	**-38.85 °C**	**234.30 K**			
CSID	452969	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.73 g/cm^3
SMILES	CC(C)(C(C)C(C)(C)C)C				
STD InChIKey	OWFKEHICSVOVAC-UHFFFAOYAN				

Melting Points

mp °C	source
-39.00	American Petroleum Institute. Research Project 44; Selected ...
-38.70	PHYSPROP

2,2,4-trimethylpentane C8H18[3, 4, 61, 64]

Compound Data



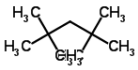
Melting point	**-107.08 °C**	**166.07 K**			
CSID	10445	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)CC(C)(C)C				
STD InChIKey	NHTMVDHEPJAVLT-UHFFFAOYAA				

Melting Points

mp °C	source
-107.00	Alfa Aesar
-107.00	American Petroleum Institute. Research Project 44; Selected ...
-107.00	Oxford University MSDS
-107.30	PHYSPROP

2,2,4,4-tetramethylpentane C9H20[4, 64]

Compound Data



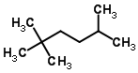
Melting point	**-66.75 °C**	**206.40 K**			
CSID	13439	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)(C)CC(C)(C)C				
STD InChIKey	GUMULFRCHLJNDY-UHFFFAOYAF				

Melting Points

mp °C	source
-67.00	American Petroleum Institute. Research Project 44; Selected ...
-66.50	PHYSPROP

2,2,5-trimethylhexane C9H20[4, 64]

Compound Data



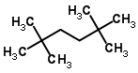
Melting point	**-105.85 °C**	**167.30 K**			
CSID	17976	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)CCC(C)(C)C				
STD InChIKey	HHOSMYBYIHNXNO-UHFFFAOYAA				

Melting Points

mp °C	source
-106.00	American Petroleum Institute. Research Project 44; Selected ...
-105.70	PHYSPROP

2,2,5,5-tetramethylhexane C10H22[4, 64]

Compound Data



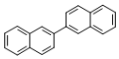
Melting point	**-12.80 °C**	**260.35 K**			
CSID	13448	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.73 g/cm^3
SMILES	CC(C)(CCC(C)(C)C)C				
STD InChIKey	HXQDUXXBVMMIKL-UHFFFAOYAZ				

Melting Points

mp °C	source
-13.00	American Petroleum Institute. Research Project 44; Selected ...
-12.60	PHYSPROP

2,2'-binaphthalene C20H14[48, 64]

Compound Data



Melting point	**187.65 °C**	**460.80 K**			
CSID	62381	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	254.3252	**H bond donors**	0	**ACD/LogP**	6.44
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	c14ccccc1ccc(c3cc2ccccc2cc3)c4				
STD InChIKey	MSBVBOUOMVTWKE-UHFFFAOYAM				

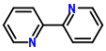
Melting Points

mp °C	source
187.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
188.30	PHYSPROP

2,2'-bipyridine C10H8N2[3, 64]

Compound Data

Melting point	**71.00 °C**	**344.15 K**			
CSID	13867714	**H bond acceptors**	2	**Rule of 5 violations**	0



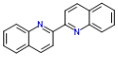
Molecular weight	156.1839	**H bond donors**	0	**ACD/LogP**	1.69
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	c1ccnc(c1)c2ccccn2				
STD InChIKey	ROFVEXUMMXZLPA-UHFFFAOYAP				

Melting Points

mp °C	source
70.00	Alfa Aesar
72.00	PHYSPROP

2,2'-biquinoline C18H12N2[3, 64]

Compound Data



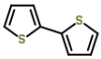
Melting point	**194.75 °C**	**467.90 K**			
CSID	8105	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	256.3013	**H bond donors**	0	**ACD/LogP**	3.82
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	n1c4c(ccc1c2nc3ccccc3cc2)cccc4				
STD InChIKey	WPTCSQBWLUUYDV-UHFFFAOYAV				

Melting Points

mp °C	source
195.00	Alfa Aesar
194.50	PHYSPROP

2,2'-bithiophene C8H6S2[3, 64]

Compound Data



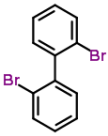
Melting point	**32.50 °C**	**305.65 K**			
CSID	61428	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	166.2632	**H bond donors**	0	**ACD/LogP**	3.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	c1cc(sc1)c2cccs2				
STD InChIKey	OHZAHWOAMVVGEL-UHFFFAOYAB				

Melting Points

mp °C	source
32.00	Alfa Aesar
33.00	PHYSPROP

2,2'-dibromobiphenyl C12H8Br2[3, 48]

Compound Data



Melting point	**80.50 °C**	**353.65 K**			
CSID	74932	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	311.9999	**H bond donors**	0	**ACD/LogP**	5.11
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.67 g/cm^3
SMILES	Brc2ccccc2c1c(Br)cccc1				
STD InChIKey	DRKHIWKXLZCAKP-UHFFFAOYAM				

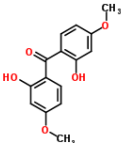
Melting Points

mp °C	source
80.00	Alfa Aesar
81.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2,2'-dihydroxy-4,4'-dimethoxybenzophenone C15H14O5[3, 64]

Compound Data

Melting point	**137.25 °C**	**410.40 K**			
CSID	8252	**H bond acceptors**	5	**Rule of 5 violations**	0



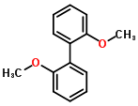
Molecular weight	274.2687	**H bond donors**	2	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1ccc(OC)cc1O)c2ccc(OC)cc2O				
STD InChIKey	SODJJEXAWOSSON-UHFFFAOYAQ				

Melting Points

mp °C	source
135.00	Alfa Aesar
139.50	PHYSPROP

2,2'-dimethoxybiphenyl C14H14O2[3, 48, 64]

Compound Data



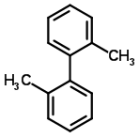
Melting point	**155.00 °C**	**428.15 K**			
CSID	531832	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	214.2598	**H bond donors**	0	**ACD/LogP**	3.31
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.06 g/cm^3
SMILES	O(c2ccccc2c1ccccc1OC)C				
STD InChIKey	VGMKUVCDINAAFC-UHFFFAOYAU				

Melting Points

mp °C	source
154.00	Alfa Aesar
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
155.00	PHYSPROP

2,2'-dimethylbiphenyl C14H14[4, 64]

Compound Data



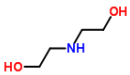
Melting point	**18.75 °C**	**291.90 K**			
CSID	11304	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	c2(c(c1ccccc1C)cccc2)C				
STD InChIKey	ABMKWMASVFVTMD-UHFFFAOYAF				

Melting Points

mp °C	source
18.00	American Petroleum Institute. Research Project 44; Selected ...
19.50	PHYSPROP

2,2'-iminodiethanol C4H11NO2[3, 61, 64]

Compound Data



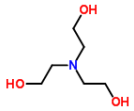
Melting point	**28.33 °C**	**301.48 K**			
CSID	13835604	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	105.1356	**H bond donors**	3	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.07 g/cm^3
SMILES	C(CO)NCCO				
STD InChIKey	ZBCBWPMODOFKDW-UHFFFAOYAO				

Melting Points

mp °C	source
29.00	Alfa Aesar
28.00	Oxford University MSDS
28.00	PHYSPROP

2,2',2''-nitrilotriethanol C6H15NO3[3, 61, 64]

Compound Data



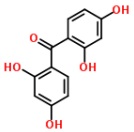
Melting point	**20.00 °C**	**293.15 K**			
CSID	13835630	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	149.1882	**H bond donors**	3	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	1.17 g/cm^3
SMILES	OCCN(CCO)CCO				
STD InChIKey	GSEJCLTVZPLZKY-UHFFFAOYAL				

Melting Points

mp °C	source
20.00	Alfa Aesar
19.50	Oxford University MSDS
20.50	PHYSPROP

2,2',4,4'-tetrahydroxybenzophenone C13H10O5[3, 64]

Compound Data



Melting point	**201.25 °C**	**474.40 K**			
CSID	8253	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	246.2155	**H bond donors**	4	**ACD/LogP**	3.16
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.53 g/cm^3
SMILES	O=C(c1ccc(O)cc1O)c2ccc(O)cc2O				
STD InChIKey	WXNRYSGJLQFHBR-UHFFFAOYAO				

Melting Points

mp °C	source
201.00	Alfa Aesar
201.50	PHYSPROP

2,3-dichloro-5,6-dicyanobenzoquinone C8Cl2N2O2[3, 64]

Compound Data

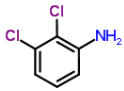
Melting point	**214.75 °C**	**487.90 K**			
CSID	6517	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	227.0038	**H bond donors**	0	**ACD/LogP**	-0.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.70 g/cm^3
SMILES	ClC=1C(=O)C(\C#N)=C(\C#N)C(=O)C=1Cl				
STD InChIKey	HZNVUJQVZSTENZ-UHFFFAOYAL				

Melting Points

mp °C	source
215.00	Alfa Aesar
214.50	PHYSPROP

2,3-dichloroaniline C6H5Cl2N[2, 3, 64]

Compound Data



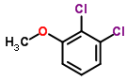
Melting point	**23.33 °C**	**296.48 K**			
CSID	21111810	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.0166	**H bond donors**	2	**ACD/LogP**	2.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Nc1cccc(Cl)c1Cl				
STD InChIKey	BRPSAOUFIJSKOT-UHFFFAOYAL				

Melting Points

mp °C	source
24.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
22.00	Alfa Aesar
24.00	PHYSPROP

2,3-dichloroanisole C7H6Cl2O[2, 3, 64]

Compound Data



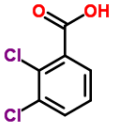
Melting point	**31.67 °C**	**304.82 K**			
CSID	15310	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	0	**ACD/LogP**	3.38
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Clc1c(OC)cccc1Cl				
STD InChIKey	HFEASCCDHUVYKU-UHFFFAOYAA				

Melting Points

mp °C	source
31.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar
32.00	PHYSPROP

2,3-dichlorobenzoic acid C7H4Cl2O2[3, 64]

Compound Data



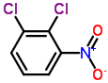
Melting point	**168.50 °C**	**441.65 K**			
CSID	5562	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	191.0115	**H bond donors**	1	**ACD/LogP**	2.92
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	Clc1c(C(=O)O)cccc1Cl				
STD InChIKey	QAOJBHRZQQDFHA-UHFFFAOYAD				

Melting Points

mp °C	source
168.00	Alfa Aesar
169.00	PHYSPROP

2,3-dichloronitrobenzene C6H3Cl2NO2[2, 3, 64]

Compound Data



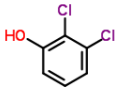
Melting point	**61.83 °C**	**334.98 K**			
CSID	21106574	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.9995	**H bond donors**	0	**ACD/LogP**	2.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3
SMILES	Clc1c(cccc1Cl)[N+](=O)[O-]				
STD InChIKey	CMVQZRLQEOAYSW-UHFFFAOYAP				

Melting Points

mp °C	source
62.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
62.00	Alfa Aesar
61.50	PHYSPROP

2,3-dichlorophenol C6H4Cl2O[2, 3, 28, 61, 64, 72]

Compound Data



Melting point	**57.67 °C**	**330.82 K**			
CSID	10857	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.0014	**H bond donors**	1	**ACD/LogP**	2.83
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	Clc1c(O)cccc1Cl				
STD InChIKey	UMPSXRYVXUPCOS-UHFFFAOYAZ				

Melting Points

mp °C	source
59.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
59.00	Alfa Aesar
58.00	CRC Handbook of Chemistry and Physics
56.00	Oxford University MSDS
58.00	PHYSPROP
56.00	Sigma-Aldrich

2,3-dichloropyridine $C_5H_3Cl_2N$[3, 64]

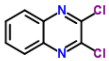
Compound Data

Melting point	**66.50 °C**	**339.65 K**			
CSID	16094	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	147.99	**H bond donors**	0	**ACD/LogP**	2.12
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	c1cc(c(nc1)Cl)Cl				
STD InChIKey	MAKFMOSBBNKPMS-UHFFFAOYAM				

Melting Points

mp °C	source
67.00	Alfa Aesar
66.00	PHYSPROP

2,3-dichloroquinoxaline $C_8H_4Cl_2N_2$[3, 61, 64]



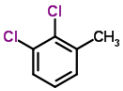
Compound Data

Melting point	**152.67 °C**	**425.82 K**			
CSID	15796	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	199.0368	**H bond donors**	0	**ACD/LogP**	2.97
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	c1ccc2c(c1)nc(c(n2)Cl)Cl				
STD InChIKey	SPSSDDOTEZKOOV-UHFFFAOYAN				

Melting Points

mp °C	source
153.00	Alfa Aesar
152.00	Oxford University MSDS
153.00	PHYSPROP

2,3-dichlorotoluene $C_7H_6Cl_2$[2, 3, 64]



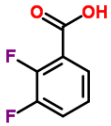
Compound Data

Melting point	**5.33 °C**	**278.48 K**			
CSID	31931	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	161.0285	**H bond donors**	0	**ACD/LogP**	3.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	Clc1c(cccc1Cl)C				
STD InChIKey	GWLKCPXYBLCEKC-UHFFFAOYAA				

Melting Points

mp °C	source
6.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
4.00	Alfa Aesar
6.00	PHYSPROP

2,3-difluorobenzoic acid $C_7H_4F_2O_2$[3, 64]



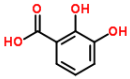
Compound Data

Melting point	**163.00 °C**	**436.15 K**			
CSID	328957	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1023	**H bond donors**	1	**ACD/LogP**	2.03
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	Fc1c(C(=O)O)cccc1F				
STD InChIKey	JLZVIWSFUPLSOR-UHFFFAOYAR				

Melting Points

mp °C	source
162.00	Alfa Aesar
164.00	PHYSPROP

2,3-dihydroxybenzoic acid $C_7H_6O_4$[3, 32, 64]



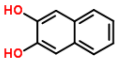
Compound Data

Melting point	**204.67 °C**	**477.82 K**			
CSID	18	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	154.1201	**H bond donors**	3	**ACD/LogP**	1.62
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.56 g/cm^3
SMILES	c1cc(c(c(c1)O)O)C(=O)O				
STD InChIKey	GLDQAMYCGOIJDV-UHFFFAOYAE				

Melting Points

mp °C	source
206.00	Alfa Aesar
204.00	DrugBank
204.00	PHYSPROP

2,3-dihydroxynaphthalene $C_{10}H_8O_2$[3, 64]



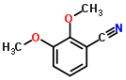
Compound Data

Melting point	**163.00 °C**	**436.15 K**			
CSID	6824	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.1693	**H bond donors**	2	**ACD/LogP**	2.11
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	Oc2cc1c(cccc1)cc2O				
STD InChIKey	JRNGUTKWMSBIBF-UHFFFAOYAQ				

Melting Points

mp °C	source
164.00	Alfa Aesar
162.00	PHYSPROP

2,3-dimethoxybenzonitrile $C_9H_9NO_2$[3, 61]



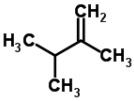
Compound Data

Melting point	**45.25 °C**	**318.40 K**			
CSID	20548	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	163.1733	**H bond donors**	0	**ACD/LogP**	1.57
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.12 g/cm^3
SMILES	N#Cc1cccc(OC)c1OC				
STD InChIKey	LBXGBNHUNHWYRM-UHFFFAOYAW				

Melting Points

mp °C	source
46.00	Alfa Aesar
44.50	Oxford University MSDS

2,3-dimethyl-1-butene C_6H_{12}[3, 4, 64]



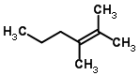
Compound Data

Melting point	**-157.10 °C**	**116.05 K**			
CSID	10775	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.69 g/cm^3
SMILES	C=C(/C)C(C)C				
STD InChIKey	OWWIWYDDISJUMY-UHFFFAOYAI				

Melting Points

mp °C	source
-157.00	Alfa Aesar
-157.00	American Petroleum Institute. Research Project 44; Selected ...
-157.30	PHYSPROP

2,3-dimethyl-2-hexene C8H16[4, 64]



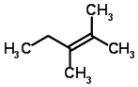
Compound Data

Melting point	**-115.05 °C**	**158.10 K**			
CSID	21998	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.53
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.73 g/cm^3
SMILES	C(=C(/C)CCC)(\C)C				
STD InChIKey	RGYAVZGBAJFMIZ-UHFFFAOYAY				

Melting Points

mp °C	source
-115.00	American Petroleum Institute. Research Project 44; Selected ...
-115.10	PHYSPROP

2,3-dimethyl-2-pentene C7H14[4, 64]



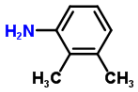
Compound Data

Melting point	**-118.15 °C**	**155.00 K**			
CSID	23718	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	4.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.71 g/cm^3
SMILES	C(=C(/C)CC)(\C)C				
STD InChIKey	WFHALSLYRWWUGH-UHFFFAOYAT				

Melting Points

mp °C	source
-118.00	American Petroleum Institute. Research Project 44; Selected ...
-118.30	PHYSPROP

2,3-dimethylaniline C8H11N[2, 3]



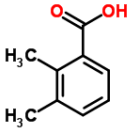
Compound Data

Melting point	**2.50 °C**	**275.65 K**			
CSID	13840647	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	Cc1cccc(N)c1C				
STD InChIKey	VVAKEQGKZNKUSU-UHFFFAOYAN				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
3.00	Alfa Aesar

2,3-dimethylbenzoic acid C9H10O2[3, 64]



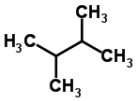
Compound Data

Melting point	**145.50 °C**	**418.65 K**			
CSID	11289	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	2.81
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	O=C(O)c1cccc(c1C)C				
STD InChIKey	RIZUCYSQUWMQLX-UHFFFAOYAN				

Melting Points

mp °C	source
145.00	Alfa Aesar
146.00	PHYSPROP

2,3-dimethylbutane C6H14[3, 4, 61, 64]



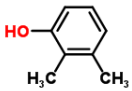
Compound Data

Melting point	**-128.70 °C**	**144.45 K**			
CSID	6340	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	86.1754	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.67 g/cm^3
SMILES	CC(C)C(C)C				
STD InChIKey	ZFFMLCVRJBZUDZ-UHFFFAOYAY				

Melting Points

mp °C	source
-129.00	Alfa Aesar
-129.00	American Petroleum Institute. Research Project 44; Selected ...
-128.00	Oxford University MSDS
-128.80	PHYSPROP

2,3-dimethylphenol C8H10O[3, 28, 31, 64, 72]



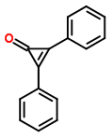
Compound Data

Melting point	**72.76 °C**	**345.91 K**			
CSID	13839151	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	Cc1cccc(O)c1C				
STD InChIKey	QWBBPBRQALCEIZ-UHFFFAOYAU				

Melting Points

mp °C	source
72.00	Alfa Aesar
72.50	CRC Handbook of Chemistry and Physics
75.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
72.80	PHYSPROP
71.50	Sigma-Aldrich

2,3-diphenyl-2-cyclopropen-1-one C15H10O[3, 64]



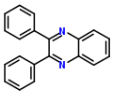
Compound Data

Melting point	**119.50 °C**	**392.65 K**			
CSID	58568	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	206.2393	**H bond donors**	0	**ACD/LogP**	3.78
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C2C(=C2\c1ccccc1)\c3ccccc3				
STD InChIKey	HCIBTBXNLVOFER-UHFFFAOYAZ				

Melting Points

mp °C	source
120.00	Alfa Aesar
119.00	PHYSPROP

2,3-diphenylquinoxaline C20H14N2[3, 61]



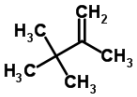
Compound Data

Melting point	**126.25 °C**	**399.40 K**			
CSID	66909	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	282.3386	**H bond donors**	0	**ACD/LogP**	4.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	n1c4ccccc4nc(c1c2ccccc2)c3ccccc3				
STD InChIKey	RSNQVABHABAKEZ-UHFFFAOYAA				

Melting Points

mp °C	source
126.00	Alfa Aesar
126.50	Oxford University MSDS

2,3,3-trimethyl-1-butene C_7H_{14}[4, 64]



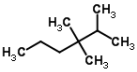
Compound Data

Melting point	**-109.95 °C**	**163.20 K**			
CSID	11179	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.71 g/cm^3
SMILES	C=C(/C)C(C)(C)C				
STD InChIKey	AUYRUAVCWOAHQN-UHFFFAOYAR				

Melting Points

mp °C	source
-110.00	American Petroleum Institute. Research Project 44; Selected ...
-109.90	PHYSPROP

2,3,3-trimethylhexane C_9H_{20}[4, 64]



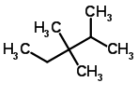
Compound Data

Melting point	**-116.90 °C**	**156.25 K**			
CSID	26065	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)C(C)(C)CCC				
STD InChIKey	DJYSEQMMCZAKGT-UHFFFAOYAV				

Melting Points

mp °C	source
-117.00	American Petroleum Institute. Research Project 44; Selected ...
-116.80	PHYSPROP

2,3,3-trimethylpentane C_8H_{18}[4, 64]



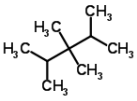
Compound Data

Melting point	**-100.95 °C**	**172.20 K**			
CSID	10742	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)C(C)(C)CC				
STD InChIKey	OKVWYBALHQFVFP-UHFFFAOYAT				

Melting Points

mp °C	source
-101.00	American Petroleum Institute. Research Project 44; Selected ...
-100.90	PHYSPROP

2,3,3,4-tetramethylpentane C_9H_{20}[4, 64]



Compound Data

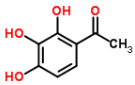
Melting point	**-102.05 °C**	**171.10 K**			
CSID	26070	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)C(C)(C)C(C)C				
STD InChIKey	JLCYYQOQSAMWTA-UHFFFAOYAI				

Melting Points

mp °C	source
-102.00	American Petroleum Institute. Research Project 44; Selected ...
-102.10	PHYSPROP

2,3,4-trihydroxyacetophenone $C_8H_8O_4$[3, 64]

Compound Data



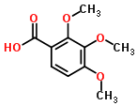
Melting point	**172.00 °C**	**445.15 K**			
CSID	10256	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	3	**ACD/LogP**	1.73
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.45 g/cm^3
SMILES	O=C(c1c(O)c(O)c(O)cc1)C				
STD InChIKey	XIROXSOOOAZHLL-UHFFFAOYAA				

Melting Points

mp °C	source
171.00	Alfa Aesar
173.00	PHYSPROP

2,3,4-trimethoxybenzoic acid C10H12O5[3, 64]

Compound Data



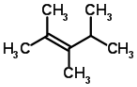
Melting point	**100.75 °C**	**373.90 K**			
CSID	10833	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	212.1993	**H bond donors**	1	**ACD/LogP**	1.38
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.22 g/cm^3
SMILES	O=C(O)c1c(OC)c(OC)c(OC)cc1				
STD InChIKey	HZNQSWJZTWOTKM-UHFFFAOYAS				

Melting Points

mp °C	source
101.00	Alfa Aesar
100.50	PHYSPROP

2,3,4-trimethyl-2-pentene C8H16[4, 64]

Compound Data



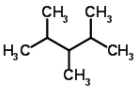
Melting point	**-113.20 °C**	**159.95 K**			
CSID	10796	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.73 g/cm^3
SMILES	C(=C(/C)C(C)C)(\C)C				
STD InChIKey	SZFRZEBLZFTODC-UHFFFAOYAT				

Melting Points

mp °C	source
-113.00	American Petroleum Institute. Research Project 44; Selected ...
-113.40	PHYSPROP

2,3,4-trimethylpentane C8H18[3, 4, 64]

Compound Data



Melting point	**-109.40 °C**	**163.75 K**			
CSID	10795	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)C(C)C(C)C				
STD InChIKey	RLPGDEORIPLBNF-UHFFFAOYAR				

Melting Points

mp °C	source
-110.00	Alfa Aesar
-109.00	American Petroleum Institute. Research Project 44; Selected ...
-109.20	PHYSPROP

2,3,4,5,6-pentafluorobenzamide C7H18N2[3, 64]

Compound Data

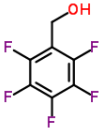
Melting point	**28.45 °C**	**301.60 K**			
CSID	62737	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.2312	**H bond donors**	4	**ACD/LogP**	0.57
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	0.86 g/cm^3
SMILES	NCCCCCCCN				
STD InChIKey	PWSKHLMYTZNYKO-UHFFFAOYAF				

Melting Points

mp °C	source
28.00	Alfa Aesar
28.90	PHYSPROP

2,3,4,5,6-pentafluorobenzyl alcohol C7H3F5O[3, 32, 64]

Compound Data



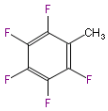
Melting point	**36.33 °C**	**309.48 K**			
CSID	9535	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	198.0901	**H bond donors**	1	**ACD/LogP**	1.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.59 g/cm^3
SMILES	Fc1c(c(F)c(F)c(F)c1F)CO				
STD InChIKey	PGJYYCIOYBZTPU-UHFFFAOYAP				

Melting Points

mp °C	source
34.00	Alfa Aesar
37.50	DrugBank
37.50	PHYSPROP

2,3,4,5,6-pentafluorotoluene C7H3F5[3, 64]

Compound Data



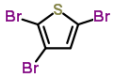
Melting point	**-29.90 °C**	**243.25 K**			
CSID	21168888	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.0907	**H bond donors**	0	**ACD/LogP**	2.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.44 g/cm^3
SMILES	Fc1c(C)c(F)c(F)c(F)c1F				
STD InChIKey	SXPRVMIZFRCAGC-UHFFFAOYAI				

Melting Points

mp °C	source
-30.00	Alfa Aesar
-29.80	PHYSPROP

2,3,5-tribromothiophene C4HBr3S[3, 64]

Compound Data



Melting point	**28.00 °C**	**301.15 K**			
CSID	69057	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	320.8277	**H bond donors**	0	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.52 g/cm^3
SMILES	Brc1sc(Br)c(Br)c1				
STD InChIKey	SKDNDSLDRLEELJ-UHFFFAOYAQ				

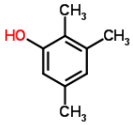
Melting Points

mp °C	source
27.00	Alfa Aesar
29.00	PHYSPROP

2,3,5-trimethylphenol C9H12O[3, 64]

Compound Data

Melting point	**93.75 °C**	**366.90 K**



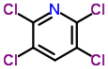
CSID	12244	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	1	**ACD/LogP**	2.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	Oc1cc(cc(c1C)C)C				
STD InChIKey	OGRAOKJKVGDSFR-UHFFFAOYAF				

Melting Points

mp °C	source
94.00	Alfa Aesar
93.50	PHYSPROP

2,3,5,6-tetrachloropyridine C5HCl4N[3, 64]

Compound Data



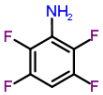
Melting point	**90.75 °C**	**363.90 K**			
CSID	16096	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	216.8801	**H bond donors**	0	**ACD/LogP**	3.38
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.66 g/cm^3
SMILES	Clc1c(Cl)nc(Cl)c(Cl)c1				
STD InChIKey	FATBKZJZAHWCSL-UHFFFAOYAH				

Melting Points

mp °C	source
91.00	Alfa Aesar
90.50	PHYSPROP

2,3,5,6-tetrafluoroaniline C6H3F4N[3, 64]

Compound Data



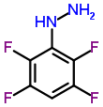
Melting point	**31.25 °C**	**304.40 K**			
CSID	21112533	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	165.0883	**H bond donors**	2	**ACD/LogP**	2.54
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	Fc1cc(F)c(F)c(N)c1F				
STD InChIKey	SPSWJTZNOXMMMV-UHFFFAOYAI				

Melting Points

mp °C	source
31.00	Alfa Aesar
31.50	PHYSPROP

2,3,5,6-tetrafluorophenylhydrazine C6H4F4N2[3, 64]

Compound Data



Melting point	**90.50 °C**	**363.65 K**			
CSID	62756	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	180.103	**H bond donors**	3	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.59 g/cm^3
SMILES	Fc1c(F)cc(F)c(F)c1NN				
STD InChIKey	TYMFVEOXNZYYTF-UHFFFAOYAD				

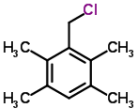
Melting Points

mp °C	source
89.00	Alfa Aesar
92.00	PHYSPROP

2,3,5,6-tetramethylbenzyl chloride C11H15Cl[3, 3, 48, 75]

Compound Data

Melting point	**70.00 °C**	**343.15 K**			
CSID	73945	**H bond acceptors**	0	**Rule of 5 violations**	0



Molecular weight	182.6898	**H bond donors**	0	**ACD/LogP**	4.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	ClCc1c(c(cc(c1C)C)C)C				
STD InChIKey	UGAPPXGBBWAIGT-UHFFFAOYAT				

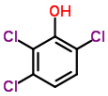
Melting Points

mp °C	source
70.00	Alfa Aesar
69.50	Alfa Aesar
70.50	TauChem
	Values not used in calculating the average melting point
168.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...[1]

1. clearly out of range JCB

2,3,6-trichlorophenol C6H3Cl3O[61, 64]

Compound Data



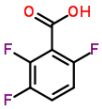
Melting point	**57.00 °C**	**330.15 K**			
CSID	13029	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	197.4464	**H bond donors**	1	**ACD/LogP**	3.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.60 g/cm^3
SMILES	Clc1c(O)c(Cl)ccc1Cl				
STD InChIKey	XGCHAIDDPMFRLJ-UHFFFAOYAK				

Melting Points

mp °C	source
56.00	Oxford University MSDS
58.00	PHYSPROP

2,3,6-trifluorobenzoic acid C7H3F3O2[3, 64]

Compound Data



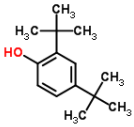
Melting point	**130.75 °C**	**403.90 K**			
CSID	453633	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	176.0927	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	Fc1c(C(=O)O)c(F)ccc1F				
STD InChIKey	MGUPHQGQNHDGNK-UHFFFAOYAZ				

Melting Points

mp °C	source
131.00	Alfa Aesar
130.50	PHYSPROP

2,4-di-t-butylphenol C14H22O[3, 61, 64]

Compound Data

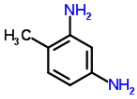


Melting point	**55.33 °C**	**328.48 K**			
CSID	7037	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	206.3239	**H bond donors**	1	**ACD/LogP**	4.86
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.93 g/cm^3
SMILES	Oc1ccc(cc1C(C)(C)C)C(C)(C)C				
STD InChIKey	ICKWICRCANNIBI-UHFFFAOYAJ				

Melting Points

mp °C	source
55.00	Alfa Aesar
54.50	Oxford University MSDS
56.50	PHYSPROP

2,4-diaminotoluene C7H10N2[2, 3, 64]



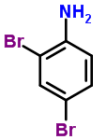
Compound Data

Melting point	**98.33 °C**	**371.48 K**			
CSID	6991	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1677	**H bond donors**	4	**ACD/LogP**	0.15
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	Nc1cc(N)c(cc1)C				
STD InChIKey	VOZKAJLKRJDJLL-UHFFFAOYAX				

Melting Points

mp °C	source
97.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
99.00	Alfa Aesar
99.00	PHYSPROP

2,4-dibromoaniline C6H5Br2N[2, 3, 64]



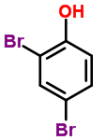
Compound Data

Melting point	**79.17 °C**	**352.32 K**			
CSID	11509	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	250.9186	**H bond donors**	2	**ACD/LogP**	3.26
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.02 g/cm^3
SMILES	Brc1cc(Br)c(N)cc1				
STD InChIKey	DYSRXWYRUJCNFI-UHFFFAOYAA				

Melting Points

mp °C	source
78.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
80.00	Alfa Aesar
79.50	PHYSPROP

2,4-dibromophenol C6H4Br2O[2, 3, 64]



Compound Data

Melting point	**38.33 °C**	**311.48 K**			
CSID	11510	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	251.9034	**H bond donors**	1	**ACD/LogP**	3.43
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.10 g/cm^3
SMILES	Brc1cc(Br)c(O)cc1				
STD InChIKey	FAXWFCTVSHEODL-UHFFFAOYAP				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
37.00	Alfa Aesar
38.00	PHYSPROP

2,4-dichloro-1-nitrobenzene C6H3Cl2NO2[2, 3, 61, 64]

Compound Data

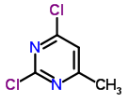
Melting point	**31.62 °C**	**304.77 K**			
CSID	21106035	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.9995	**H bond donors**	0	**ACD/LogP**	3.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3
SMILES	O=[N+]([O-])c1ccc(Cl)cc1Cl				
STD InChIKey	QUIMTLZDMCNYGY-UHFFFAOYAW				

Melting Points

mp °C	source
31.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
31.00	Alfa Aesar
30.50	Oxford University MSDS

34.00	PHYSPROP

2,4-dichloro-6-methylpyrimidine C5H4Cl2N2[3, 64]



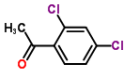
Compound Data

Melting point	**46.25 °C**	**319.40 K**			
CSID	71784	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	163.0047	**H bond donors**	0	**ACD/LogP**	1.61
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	Cc1cc(nc(n1)Cl)Cl				
STD InChIKey	BTLKROSJMNFSQZ-UHFFFAOYAF				

Melting Points

mp °C	source
46.00	Alfa Aesar
46.50	PHYSPROP

2,4-dichloroacetophenone C8H6Cl2O[2, 3, 64]



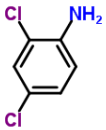
Compound Data

Melting point	**33.50 °C**	**306.65 K**			
CSID	21106529	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	189.0386	**H bond donors**	0	**ACD/LogP**	2.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	O=C(C)c1ccc(Cl)cc1Cl				
STD InChIKey	XMCRWEBERCXJCH-UHFFFAOYAG				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
33.00	Alfa Aesar
33.50	PHYSPROP

2,4-dichloroaniline C6H5Cl2N[2, 3, 64]



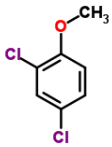
Compound Data

Melting point	**61.83 °C**	**334.98 K**			
CSID	13860817	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.0166	**H bond donors**	2	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Clc1cc(Cl)c(N)cc1				
STD InChIKey	KQCMTOWTPBNWDB-UHFFFAOYAS				

Melting Points

mp °C	source
61.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
61.00	Alfa Aesar
63.50	PHYSPROP

2,4-dichloroanisole C7H6Cl2O[3, 64]



Compound Data

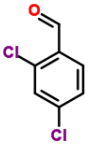
Melting point	**27.25 °C**	**300.40 K**			
CSID	10648	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	0	**ACD/LogP**	3.38
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Clc1cc(Cl)ccc1OC				
STD InChIKey	CICQUFBZCADHHX-UHFFFAOYAA				

Melting Points

mp °C	source
26.00	Alfa Aesar

28.50	PHYSPROP

2,4-dichlorobenzaldehyde C7H4Cl2O[2, 3, 64]



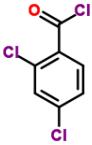
Compound Data

Melting point	**72.00 °C**	**345.15 K**			
CSID	12830	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.0121	**H bond donors**	0	**ACD/LogP**	2.91
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	O=Cc1ccc(Cl)cc1Cl				
STD InChIKey	YSFBEAASFUWWHU-UHFFFAOYAZ				

Melting Points

mp °C	source
73.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
71.00	Alfa Aesar
72.00	PHYSPROP

2,4-dichlorobenzoyl chloride C7H3Cl3O[3, 64]



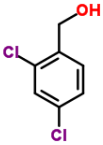
Compound Data

Melting point	**17.25 °C**	**290.40 K**			
CSID	60012	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	209.4571	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.50 g/cm^3
SMILES	O=C(Cl)c1ccc(Cl)cc1Cl				
STD InChIKey	CEOCVKWBUWKBKA-UHFFFAOYAU				

Melting Points

mp °C	source
18.00	Alfa Aesar
16.50	PHYSPROP

2,4-dichlorobenzyl alcohol C7H6Cl2O[3, 64]



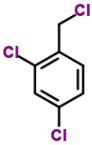
Compound Data

Melting point	**59.25 °C**	**332.40 K**			
CSID	14918	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	1	**ACD/LogP**	2.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	Clc1cc(Cl)ccc1CO				
STD InChIKey	DBHODFSFBXJZNY-UHFFFAOYAI				

Melting Points

mp °C	source
59.00	Alfa Aesar
59.50	PHYSPROP

2,4-dichlorobenzyl chloride C7H5Cl3[3, 31, 64]



Compound Data

Melting point	**-2.87 °C**	**270.28 K**			
CSID	6942	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	195.4736	**H bond donors**	0	**ACD/LogP**	3.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	ClCc1ccc(Cl)cc1Cl				
STD InChIKey	IRSVDHPYXFLLDS-UHFFFAOYAR				

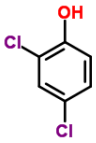
Melting Points

mp °C	source
-3.00	Alfa Aesar
-3.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...

-2.60	PHYSPROP

2,4-dichlorophenol C6H4Cl2O[2, 3, 64, 70]

Compound Data



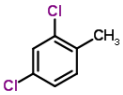
Melting point	**43.75 °C**	**316.90 K**			
CSID	8140	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.0014	**H bond donors**	1	**ACD/LogP**	3.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	Clc1cc(Cl)c(O)cc1				
STD InChIKey	HFZWRUODUSTPEG-UHFFFAOYAU				

Melting Points

mp °C	source
43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
42.00	Alfa Aesar
45.00	PHYSPROP
45.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

2,4-dichlorotoluene C7H6Cl2[3, 64]

Compound Data



Melting point	**-13.25 °C**	**259.90 K**			
CSID	21111905	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	161.0285	**H bond donors**	0	**ACD/LogP**	3.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	Clc1cc(Cl)c(C)cc1				
STD InChIKey	FUNUTBJJKQIVSY-UHFFFAOYAA				

Melting Points

mp °C	source
-13.00	Alfa Aesar
-13.50	PHYSPROP

2,4-difluoro-1-nitrobenzene C6H3F2NO2[3, 61, 64]

Compound Data

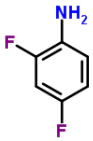
Melting point	**9.60 °C**	**282.75 K**			
CSID	21106036	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	159.0903	**H bond donors**	0	**ACD/LogP**	1.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.45 g/cm^3
SMILES	O=[N+]([O-])c1ccc(F)cc1F				
STD InChIKey	RJXOVESYJFXCGI-UHFFFAOYAO				

Melting Points

mp °C	source
10.00	Alfa Aesar
9.00	Oxford University MSDS
9.80	PHYSPROP

2,4-difluoroaniline C6H5F2N[3, 61, 64]

Compound Data



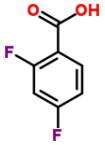
Melting point	**-7.67 °C**	**265.48 K**			
CSID	9328	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.1074	**H bond donors**	2	**ACD/LogP**	1.52
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Fc1ccc(N)c(F)c1				
STD InChIKey	CEPCPXLLFXPZGW-UHFFFAOYAI				

Melting Points

mp °C	source

-8.00	Alfa Aesar
-7.50	Oxford University MSDS
-7.50	PHYSPROP

2,4-difluorobenzoic acid C7H4F2O2[3, 64]



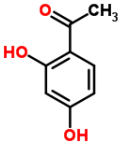
Compound Data

Melting point	**188.50 °C**	**461.65 K**			
CSID	66716	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1023	**H bond donors**	1	**ACD/LogP**	2.07
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	O=C(O)c1ccc(F)cc1F				
STD InChIKey	NJYBIFYEWYWYAN-UHFFFAOYAW				

Melting Points

mp °C	source
188.00	Alfa Aesar
189.00	PHYSPROP

2,4-dihydroxyacetophenone C8H8O3[3, 64]



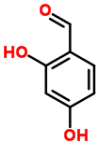
Compound Data

Melting point	**145.00 °C**	**418.15 K**			
CSID	6724	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	1.74
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1ccc(O)cc1O)C				
STD InChIKey	SULYEHHGGXARJS-UHFFFAOYAF				

Melting Points

mp °C	source
144.00	Alfa Aesar
146.00	PHYSPROP

2,4-dihydroxybenzaldehyde C7H6O3[2, 3, 48, 61, 64]



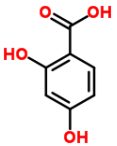
Compound Data

Melting point	**135.60 °C**	**408.75 K**			
CSID	6943	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	138.1207	**H bond donors**	2	**ACD/LogP**	1.38
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.41 g/cm^3
SMILES	O=Cc1ccc(O)cc1O				
STD InChIKey	IUNJCFABHJZSKB-UHFFFAOYAX				

Melting Points

mp °C	source
135.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
136.00	Alfa Aesar
136.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
136.00	Oxford University MSDS
135.00	PHYSPROP

2,4-dihydroxybenzoic acid C7H6O4[2, 32]



Compound Data

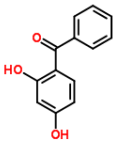
Melting point	**225.50 °C**	**498.65 K**			
CSID	1446	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	154.1201	**H bond donors**	3	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.56 g/cm^3
SMILES	c1cc(c(cc1O)O)C(=O)O				
STD InChIKey	UIAFKZKHHVMJGS-UHFFFAOYAR				

Melting Points

mp °C	source
225.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
226.00	DrugBank

2,4-dihydroxybenzophenone C13H10O3[3, 64]

Compound Data



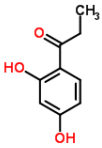
Melting point	**145.00 °C**	**418.15 K**			
CSID	8254	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.2167	**H bond donors**	2	**ACD/LogP**	3.17
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.30 g/cm^3
SMILES	O=C(c1ccc(O)cc1O)c2ccccc2				
STD InChIKey	ZXDDPOHVAMWLBH-UHFFFAOYAB				

Melting Points

mp °C	source
146.00	Alfa Aesar
144.00	PHYSPROP

2,4-dihydroxypropiophenone C9H10O3[3, 64]

Compound Data



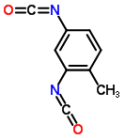
Melting point	**99.50 °C**	**372.65 K**			
CSID	72148	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	2	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.24 g/cm^3
SMILES	O=C(c1ccc(O)cc1O)CC				
STD InChIKey	LLBBBYLDTDJMNU-UHFFFAOYAE				

Melting Points

mp °C	source
100.00	Alfa Aesar
99.00	PHYSPROP

2,4-diisocyanato-1-methylbenzene C9H6N2O2[3, 61, 64, 64, 64]

Compound Data



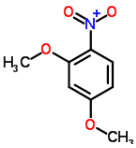
Melting point	**20.40 °C**	**293.55 K**			
CSID	13835351	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1561	**H bond donors**	0	**ACD/LogP**	3.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	Cc1ccc(cc1\N=C=O)\N=C=O				
STD InChIKey	DVKJHBMWWAPEIU-UHFFFAOYAL				

Melting Points

mp °C	source
21.00	Alfa Aesar
20.50	Oxford University MSDS
20.50	PHYSPROP
20.00	PHYSPROP
20.00	PHYSPROP

2,4-dimethoxy-1-nitrobenzene C8H9NO4[3, 64]

Compound Data



Melting point	**75.25 °C**	**348.40 K**			
CSID	70990	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	183.1614	**H bond donors**	0	**ACD/LogP**	1.69
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	[O-][N+](=O)c1ccc(OC)cc1OC				

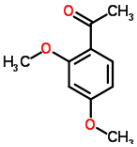
STD InChIKey	XXWIYOBCHKCWNT-UHFFFAOYAL

Melting Points

mp °C	source
74.00	Alfa Aesar
76.50	PHYSPROP

2,4-dimethoxyacetophenone C10H12O3[2, 3]

Compound Data



Melting point	**40.50 °C**	**313.65 K**			
CSID	63208	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	0	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	O=C(c1ccc(OC)cc1OC)C				
STD InChIKey	VQTDPCRSXHFMOL-UHFFFAOYAO				

Melting Points

mp °C	source
41.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
40.00	Alfa Aesar

2,4-dimethoxyaniline C8H11NO2[3, 61, 64]

Compound Data

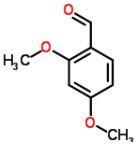
Melting point	**34.00 °C**	**307.15 K**			
CSID	16685	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	153.1784	**H bond donors**	2	**ACD/LogP**	0.78
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O(c1cc(OC)ccc1N)C				
STD InChIKey	GEQNZVKIDIPGCO-UHFFFAOYAU				

Melting Points

mp °C	source
35.00	Alfa Aesar
33.50	Oxford University MSDS
33.50	PHYSPROP

2,4-dimethoxybenzaldehyde C9H10O3[2, 3, 64]

Compound Data



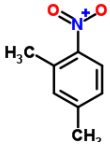
Melting point	**71.00 °C**	**344.15 K**			
CSID	62390	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	0	**ACD/LogP**	1.66
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=Cc1ccc(OC)cc1OC				
STD InChIKey	LWRSYTXEQUUTKW-UHFFFAOYAQ				

Melting Points

mp °C	source
72.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
69.00	Alfa Aesar
72.00	PHYSPROP

2,4-dimethyl-1-nitrobenzene C8H9NO2[3, 61, 64]

Compound Data



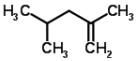
Melting point	**7.33 °C**	**280.48 K**			
CSID	6725	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	O=[N+]([O-])c1ccc(cc1C)C				

STD InChIKey	BBUPBICWUURTNP-UHFFFAOYAF

Melting Points

mp °C	source
6.00	Alfa Aesar
7.00	Oxford University MSDS
9.00	PHYSPROP

2,4-dimethyl-1-pentene C7H14[4, 64]



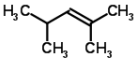
Compound Data

Melting point	**-124.05 °C**	**149.10 K**			
CSID	15794	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.70 g/cm^3
SMILES	C=C(/C)CC(C)C				
STD InChIKey	LXQPBCHJNIOMQU-UHFFFAOYAS				

Melting Points

mp °C	source
-124.00	American Petroleum Institute. Research Project 44; Selected ...
-124.10	PHYSPROP

2,4-dimethyl-2-pentene C7H14[4, 64]



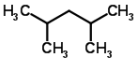
Compound Data

Melting point	**-127.85 °C**	**145.30 K**			
CSID	11757	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.79
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.71 g/cm^3
SMILES	C(=C\C(C)C)(\C)C				
STD InChIKey	VVCFYASOGFVJFN-UHFFFAOYAT				

Melting Points

mp °C	source
-128.00	American Petroleum Institute. Research Project 44; Selected ...
-127.70	PHYSPROP

2,4-dimethylpentane C7H16[3, 4, 64]



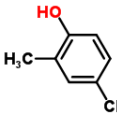
Compound Data

Melting point	**-120.63 °C**	**152.52 K**			
CSID	7619	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.2019	**H bond donors**	0	**ACD/LogP**	4.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.69 g/cm^3
SMILES	CC(C)CC(C)C				
STD InChIKey	BZHMBWZPUJHVEE-UHFFFAOYAW				

Melting Points

mp °C	source
-123.00	Alfa Aesar
-119.00	American Petroleum Institute. Research Project 44; Selected ...
-119.90	PHYSPROP

2,4-dimethylphenol C8H10O[3, 31, 64]



Compound Data

Melting point	**24.50 °C**	**297.65 K**			
CSID	13839123	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	Cc1ccc(O)c(C)c1				

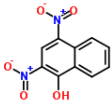
STD InChIKey	KUFFULVDNCHOFZ-UHFFFAOYAC

Melting Points

mp °C	source
22.00	Alfa Aesar
27.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
24.50	PHYSPROP

2,4-dinitro-1-naphthol C10H6N2O5[3, 61, 64]

Compound Data



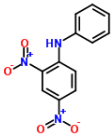
Melting point	**131.50 °C**	**404.65 K**			
CSID	11309	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	234.165	**H bond donors**	1	**ACD/LogP**	2.97
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.61 g/cm^3
SMILES	[O-][N+](=O)c2c1ccccc1c(O)c(c2)[N+]([O-])=O				
STD InChIKey	FFRBMBIXVSCUFS-UHFFFAOYAH				

Melting Points

mp °C	source
132.00	Alfa Aesar
131.50	Oxford University MSDS
131.00	PHYSPROP

2,4-dinitro-N-phenylaniline C12H9N3O4[61, 64]

Compound Data



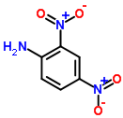
Melting point	**159.50 °C**	**432.65 K**			
CSID	13153	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	259.2176	**H bond donors**	1	**ACD/LogP**	4.11
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.45 g/cm^3
SMILES	[O-][N+](=O)c2ccc(Nc1ccccc1)c(c2)[N+]([O-])=O				
STD InChIKey	RHTVQEPJVKUMPI-UHFFFAOYAH				

Melting Points

mp °C	source
160.00	Oxford University MSDS
159.00	PHYSPROP

2,4-dinitroaniline C6H5N3O4[2, 3, 61, 64]

Compound Data



Melting point	**177.88 °C**	**451.02 K**			
CSID	7045	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	183.1216	**H bond donors**	2	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.59 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1N)[N+]([O-])=O				
STD InChIKey	LXQOQPGNCGEELI-UHFFFAOYAK				

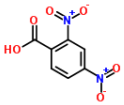
Melting Points

mp °C	source
177.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
178.00	Alfa Aesar
176.50	Oxford University MSDS
180.00	PHYSPROP

2,4-dinitrobenzoic acid C7H4N2O6[3, 64]

Compound Data

Melting point	**181.50 °C**	**454.65 K**			
CSID	11387	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	212.1165	**H bond donors**	1	**ACD/LogP**	1.49



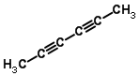
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.69 g/cm
SMILES	O=[N+]([O-])c1cc(ccc1C(=O)O)[N+]([O-])=O				
STD InChIKey	ZIIGSRYPZWDGBT-UHFFFAOYAK				

Melting Points

mp °C	source
181.00	Alfa Aesar
182.00	PHYSPROP

2,4-hexadiyne C6H6[3, 64]

Compound Data



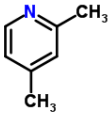
Melting point	**67.40 °C**	**340.55 K**			
CSID	121383	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	78.1118	**H bond donors**	0	**ACD/LogP**	2.24
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.83 g/cm^3
SMILES	C(#CC#CC)C				
STD InChIKey	PCTCNWZFDASPLA-UHFFFAOYAB				

Melting Points

mp °C	source
67.00	Alfa Aesar
67.80	PHYSPROP

2,4-lutidine C7H9N[3, 64]

Compound Data



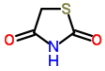
Melting point	**-62.00 °C**	**211.15 K**			
CSID	21132380	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.93 g/cm^3
SMILES	Cc1ccnc(C)c1				
STD InChIKey	JYYNAJVZFGKDEQ-UHFFFAOYAI				

Melting Points

mp °C	source
-60.00	Alfa Aesar
-64.00	PHYSPROP

2,4-thiazolidinedione C3H3NO2S[3, 64]

Compound Data



Melting point	**126.50 °C**	**399.65 K**			
CSID	5242	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	117.1264	**H bond donors**	1	**ACD/LogP**	-0.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.52 g/cm^3
SMILES	O=C1NC(=O)SC1				
STD InChIKey	ZOBPZXTWZATXDG-UHFFFAOYAD				

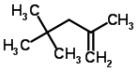
Melting Points

mp °C	source
125.00	Alfa Aesar
128.00	PHYSPROP

2,4,4-trimethyl-1-pentene C8H16[3, 4, 61, 64]

Compound Data

Melting point	**-93.62 °C**	**179.52 K**			
CSID	7580	**H bond acceptors**	0	**Rule of 5 violations**	0



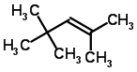
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.72 g/cm^3
SMILES	C=C(/C)CC(C)(C)C				
STD InChIKey	FXNDIJDIPNCZQJ-UHFFFAOYAF				

Melting Points

mp °C	source
-94.00	Alfa Aesar
-93.00	American Petroleum Institute. Research Project 44; Selected ...
-94.00	Oxford University MSDS
-93.50	PHYSPROP

2,4,4-trimethyl-2-pentene C8H16[3, 4, 64]

Compound Data



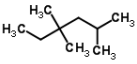
Melting point	**-106.10 °C**	**167.05 K**			
CSID	7581	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.73 g/cm^3
SMILES	C(=C\C(C)(C)C)(\C)C				
STD InChIKey	LAAVYEUJEMRIGF-UHFFFAOYAG				

Melting Points

mp °C	source
-106.00	Alfa Aesar
-106.00	American Petroleum Institute. Research Project 44; Selected ...
-106.30	PHYSPROP

2,4,4-trimethylhexane C9H20[4, 64]

Compound Data



Melting point	**-113.20 °C**	**159.95 K**			
CSID	26066	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)CC(C)(C)CC				
STD InChIKey	SVEMKBCPZYWEPH-UHFFFAOYAX				

Melting Points

mp °C	source
-113.00	American Petroleum Institute. Research Project 44; Selected ...
-113.40	PHYSPROP

2,4,5-trichloroaniline C6H4Cl3N[3, 64]

Compound Data

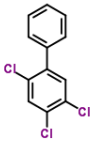
Melting point	**95.25 °C**	**368.40 K**			
CSID	21111772	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.4617	**H bond donors**	2	**ACD/LogP**	3.42
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	Nc1cc(Cl)c(Cl)cc1Cl				
STD InChIKey	GUMCAKKKNKYFEB-UHFFFAOYAK				

Melting Points

mp °C	source
94.00	Alfa Aesar
96.50	PHYSPROP

2,4,5-trichlorobiphenyl C12H7Cl3[64, 70]

Compound Data



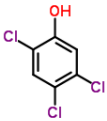
Melting point	**76.15 °C**	**349.30 K**			
CSID	25605	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	257.543	**H bond donors**	0	**ACD/LogP**	5.41
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	Clc2cc(c1ccccc1)c(Cl)cc2Cl				
STD InChIKey	VGVIKVCCUATMNG-UHFFFAOYAG				

Melting Points

mp °C	source
76.30	PHYSPROP
76.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

2,4,5-trichlorophenol C6H3Cl3O[28, 56, 64, 72, 72]

Compound Data



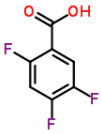
Melting point	**67.70 °C**	**340.85 K**			
CSID	7001	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	197.4464	**H bond donors**	1	**ACD/LogP**	3.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.60 g/cm^3
SMILES	Clc1cc(O)c(Cl)cc1Cl				
STD InChIKey	LHJGJYXLEPZJPM-UHFFFAOYAR				

Melting Points

mp °C	source
69.00	CRC Handbook of Chemistry and Physics
67.00	Merck Index
69.00	PHYSPROP
65.50	Sigma-Aldrich
68.00	Sigma-Aldrich

2,4,5-trifluorobenzoic acid C7H3F3O2[3, 64]

Compound Data



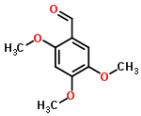
Melting point	**99.00 °C**	**372.15 K**			
CSID	454604	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	176.0927	**H bond donors**	1	**ACD/LogP**	2.31
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	Fc1cc(C(=O)O)c(F)cc1F				
STD InChIKey	AKAMNXFLKYKFOJ-UHFFFAOYAF				

Melting Points

mp °C	source
98.00	Alfa Aesar
100.00	PHYSPROP

2,4,5-trimethoxybenzaldehyde C10H12O4[2, 3, 64]

Compound Data

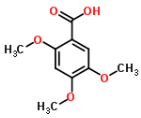


Melting point	**113.67 °C**	**386.82 K**			
CSID	19331	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	196.1999	**H bond donors**	0	**ACD/LogP**	1.62
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	O=Cc1c(OC)cc(OC)c(OC)c1				
STD InChIKey	IAJBQAYHSQIQRE-UHFFFAOYAN				

Melting Points

mp °C	source
114.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
113.00	Alfa Aesar
114.00	PHYSPROP

2,4,5-trimethoxybenzoic acid $C_{10}H_{12}O_5$[3, 64]



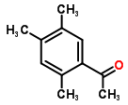
Compound Data

Melting point	**144.50 °C**	**417.65 K**			
CSID	9856	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	212.1993	**H bond donors**	1	**ACD/LogP**	1.52
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.22 g/cm^3
SMILES	O=C(O)c1c(OC)cc(OC)c(OC)c1				
STD InChIKey	KVZUCOGWKYOPID-UHFFFAOYAF				

Melting Points

mp °C	source
144.00	Alfa Aesar
145.00	PHYSPROP

2,4,5-trimethylacetophenone $C_{11}H_{14}O$[3, 64]



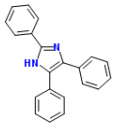
Compound Data

Melting point	**10.25 °C**	**283.40 K**			
CSID	21159574	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.2283	**H bond donors**	0	**ACD/LogP**	3.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.95 g/cm^3
SMILES	Cc1cc(C(C)=O)c(C)cc1C				
STD InChIKey	GENBEGZNCBFHSU-UHFFFAOYAI				

Melting Points

mp °C	source
10.00	Alfa Aesar
10.50	PHYSPROP

2,4,5-triphenylimidazole $C_{21}H_{16}N_2$[3, 64]



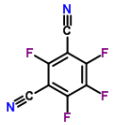
Compound Data

Melting point	**275.50 °C**	**548.65 K**			
CSID	9815	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	296.3651	**H bond donors**	1	**ACD/LogP**	4.94
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	n1c(c(nc1c2ccccc2)c3ccccc3)c4ccccc4				
STD InChIKey	RNIPJYFZGXJSDD-UHFFFAOYAN				

Melting Points

mp °C	source
276.00	Alfa Aesar
275.00	PHYSPROP

2,4,5,6-tetrafluoroisophthalonitrile $C_8F_4N_2$[3, 61]



Compound Data

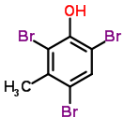
Melting point	**78.00 °C**	**351.15 K**			
CSID	528656	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.0926	**H bond donors**	0	**ACD/LogP**	-0.27
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.54 g/cm^3
SMILES	Fc1c(C#N)c(F)c(C#N)c(F)c1F				
STD InChIKey	WVHMPQKZPHOCRD-UHFFFAOYAL				

Melting Points

mp °C	source
77.00	Alfa Aesar
79.00	Oxford University MSDS

2,4,6-tribromo-3-methylphenol $C_7H_5Br_3O$[3, 64]

Compound Data



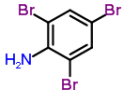
Melting point	**83.00 °C**	**356.15 K**			
CSID	19526	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	344.826	**H bond donors**	1	**ACD/LogP**	4.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.26 g/cm^3
SMILES	Brc1c(c(Br)cc(Br)c1O)C				
STD InChIKey	QKHROXOPRBWBDD-UHFFFAOYAW				

Melting Points

mp °C	source
82.00	Alfa Aesar
84.00	PHYSPROP

2,4,6-tribromoaniline C6H4Br3N[3, 61, 64]

Compound Data



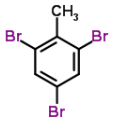
Melting point	**121.00 °C**	**394.15 K**			
CSID	21106171	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	329.8147	**H bond donors**	2	**ACD/LogP**	4.42
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.35 g/cm^3
SMILES	Brc1cc(Br)cc(Br)c1N				
STD InChIKey	GVPODVKBTHCGFU-UHFFFAOYAV				

Melting Points

mp °C	source
120.00	Alfa Aesar
121.00	Oxford University MSDS
122.00	PHYSPROP

2,4,6-tribromotoluene C7H5Br3[3, 64]

Compound Data



Melting point	**69.50 °C**	**342.65 K**			
CSID	31264	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	328.8266	**H bond donors**	0	**ACD/LogP**	4.85
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.13 g/cm^3
SMILES	Brc1cc(Br)cc(Br)c1C				
STD InChIKey	BFRIZWKDNUHPHL-UHFFFAOYAD				

Melting Points

mp °C	source
69.00	Alfa Aesar
70.00	PHYSPROP

2,4,6-trichloroaniline C6H4Cl3N[3, 61, 64]

Compound Data

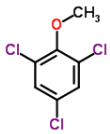
Melting point	**76.50 °C**	**349.65 K**			
CSID	11961	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.4617	**H bond donors**	2	**ACD/LogP**	3.74
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	Clc1cc(Cl)cc(Cl)c1N				
STD InChIKey	NATVSFWWYVJTAZ-UHFFFAOYAL				

Melting Points

mp °C	source
77.00	Alfa Aesar
74.00	Oxford University MSDS
78.50	PHYSPROP

2,4,6-trichloroanisole C7H5Cl3O[61, 64]

Compound Data



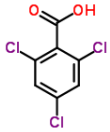
Melting point	**61.25 °C**	**334.40 K**			
CSID	6620	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	211.473	**H bond donors**	0	**ACD/LogP**	3.95
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.42 g/cm^3
SMILES	Clc1cc(Cl)cc(Cl)c1OC				
STD InChIKey	WCVOGSZTONGSQY-UHFFFAOYAT				

Melting Points

mp °C	source
61.00	Oxford University MSDS
61.50	PHYSPROP

2,4,6-trichlorobenzoic acid C7H3Cl3O2[3, 64]

Compound Data



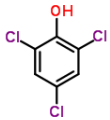
Melting point	**162.50 °C**	**435.65 K**			
CSID	5561	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	225.4565	**H bond donors**	1	**ACD/LogP**	2.98
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.64 g/cm^3
SMILES	O=C(O)c1c(Cl)cc(Cl)cc1Cl				
STD InChIKey	RAFFVQBMVYYTQS-UHFFFAOYAY				

Melting Points

mp °C	source
163.00	Alfa Aesar
162.00	PHYSPROP

2,4,6-trichlorophenol C6H3Cl3O[3, 28, 56, 61, 64, 70, 72]

Compound Data



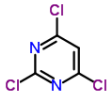
Melting point	**68.14 °C**	**341.29 K**			
CSID	21106172	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	197.4464	**H bond donors**	1	**ACD/LogP**	3.77
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.60 g/cm^3
SMILES	c1c(cc(c(c1Cl)O)Cl)Cl				
STD InChIKey	LINPIYWFGCPVIE-UHFFFAOYAP				

Melting Points

mp °C	source
66.00	Alfa Aesar
69.00	CRC Handbook of Chemistry and Physics
69.00	Merck Index
69.00	Oxford University MSDS
69.00	PHYSPROP
70.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
65.00	Sigma-Aldrich

2,4,6-trichloropyrimidine C4HCl3N2[3, 64]

Compound Data

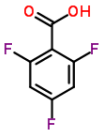


Melting point	**22.75 °C**	**295.90 K**			
CSID	69792	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	183.4231	**H bond donors**	0	**ACD/LogP**	1.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.64 g/cm^3
SMILES	c1c(nc(nc1Cl)Cl)Cl				
STD InChIKey	DPVIABCMTHHTGB-UHFFFAOYAK				

Melting Points

mp °C	source
23.00	Alfa Aesar
22.50	PHYSPROP

2,4,6-trifluorobenzoic acid C7H3F3O2[3, 64]



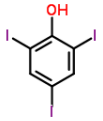
Compound Data

Melting point	**142.00 °C**	**415.15 K**			
CSID	453910	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	176.0927	**H bond donors**	1	**ACD/LogP**	2.11
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	O=C(O)c1c(F)cc(F)cc1F				
STD InChIKey	SJZATRRXUILGHH-UHFFFAOYAK				

Melting Points

mp °C	source
141.00	Alfa Aesar
143.00	PHYSPROP

2,4,6-triiodophenol C6H3I3O[2, 3, 64]



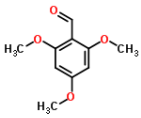
Compound Data

Melting point	**158.60 °C**	**431.75 K**			
CSID	11369	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	471.8008	**H bond donors**	1	**ACD/LogP**	3.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	3.06 g/cm^3
SMILES	Ic1cc(I)c(O)c(I)c1				
STD InChIKey	VAPDZNUFNKUROY-UHFFFAOYAZ				

Melting Points

mp °C	source
158.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
158.00	Alfa Aesar
159.80	PHYSPROP

2,4,6-trimethoxybenzaldehyde C10H12O4[2, 3, 3]



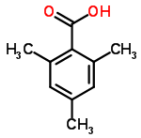
Compound Data

Melting point	**120.33 °C**	**393.48 K**			
CSID	63211	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	196.1999	**H bond donors**	0	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	O=Cc1c(OC)cc(OC)cc1OC				
STD InChIKey	CRBZVDLXAIFERF-UHFFFAOYAL				

Melting Points

mp °C	source
120.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
120.00	Alfa Aesar
121.00	Alfa Aesar

2,4,6-trimethylbenzoic acid C10H12O2[3, 48, 64]



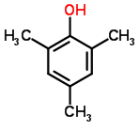
Compound Data

Melting point	**153.33 °C**	**426.48 K**			
CSID	9779	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	1	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	O=C(O)c1c(cc(cc1C)C)C				
STD InChIKey	FFFIRKXTFQCCKJ-UHFFFAOYAZ				

Melting Points

mp °C	source
154.00	Alfa Aesar
152.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
154.00	PHYSPROP

2,4,6-trimethylphenol C9H12O[3, 64]



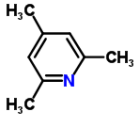
Compound Data

Melting point	**72.50 °C**	**345.65 K**			
CSID	10248	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	1	**ACD/LogP**	2.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	Oc1c(cc(cc1C)C)C				
STD InChIKey	BPRYUXCVCCNUFE-UHFFFAOYAC				

Melting Points

mp °C	source
72.00	Alfa Aesar
73.00	PHYSPROP

2,4,6-trimethylpyridine C8H11N[3, 61, 64]



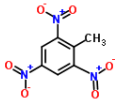
Compound Data

Melting point	**-45.00 °C**	**228.15 K**			
CSID	21106174	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	0	**ACD/LogP**	2.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.92 g/cm^3
SMILES	Cc1cc(C)cc(C)n1				
STD InChIKey	BWZVCCNYKMEVEX-UHFFFAOYAX				

Melting Points

mp °C	source
-43.00	Alfa Aesar
-46.00	Oxford University MSDS
-46.00	PHYSPROP

2,4,6-trinitrotoluene C7H5N3O6[61, 64]



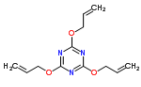
Compound Data

Melting point	**80.05 °C**	**353.20 K**			
CSID	8073	**H bond acceptors**	9	**Rule of 5 violations**	0
Molecular weight	227.1311	**H bond donors**	0	**ACD/LogP**	1.59
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.61 g/cm^3
SMILES	Cc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	SPSSULHKWOKEEL-UHFFFAOYAZ				

Melting Points

mp °C	source
80.00	Oxford University MSDS
80.10	PHYSPROP

2,4,6-tris(allyloxy)-1,3,5-triazine C12H15N3O3[3, 61, 64]



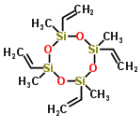
Compound Data

Melting point	**26.67 °C**	**299.82 K**			
CSID	7274	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	249.2658	**H bond donors**	0	**ACD/LogP**	2.81
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.10 g/cm^3
SMILES	O(c1nc(nc(OC\C=C)n1)OC\C=C)C/C=C				
STD InChIKey	BJELTSYBAHKXRW-UHFFFAOYAX				

Melting Points

mp °C	source
27.00	Alfa Aesar
26.00	Oxford University MSDS
27.00	PHYSPROP

2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane C12H24O4Si4[3, 64]



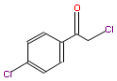
Compound Data

Melting point	**-43.25 °C**	**229.90 K**			
CSID	68224	**H bond acceptors**	4	**Rule of 5 violations**	NA
Molecular weight	344.6586	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.96 g/cm^3
SMILES	O1[Si](O[Si](O[Si]1(\C=C)C)(\C=C)C)(\C=C)C)(\C=C)C				
STD InChIKey	VMAWODUEPLAHOE-UHFFFAOYAO				

Melting Points

mp °C	source
-43.00	Alfa Aesar
-43.50	PHYSPROP

2,4'-dichloroacetophenone C8H6Cl2O[3, 64]



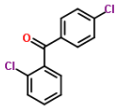
Compound Data

Melting point	**101.25 °C**	**374.40 K**			
CSID	21170959	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	189.0386	**H bond donors**	0	**ACD/LogP**	2.53
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=C(CCl)c1ccc(Cl)cc1				
STD InChIKey	FWDFNLVLIXAOMX-UHFFFAOYAS				

Melting Points

mp °C	source
101.00	Alfa Aesar
101.50	PHYSPROP

2,4'-dichlorobenzophenone C13H8Cl2O[3, 64]



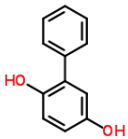
Compound Data

Melting point	**66.00 °C**	**339.15 K**			
CSID	59928	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	251.108	**H bond donors**	0	**ACD/LogP**	4.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=C(c1ccccc1Cl)c2ccc(Cl)cc2				
STD InChIKey	YXMYPHLWXBXNFF-UHFFFAOYAB				

Melting Points

mp °C	source
65.00	Alfa Aesar
67.00	PHYSPROP

2,5-biphenyldiol C12H10O2[3, 64]



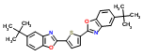
Compound Data

Melting point	**101.75 °C**	**374.90 K**			
CSID	13493	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	2	**ACD/LogP**	2.09
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	Oc2ccc(O)cc2c1ccccc1				
STD InChIKey	XCZKKZXWDBOGPA-UHFFFAOYAQ				

Melting Points

mp °C	source
101.00	Alfa Aesar
102.50	PHYSPROP

2,5-bis(5-t-butyl-2-benzoxazolyl)thiophene C26H26N2O2S[3, 61]



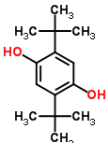
Compound Data

Melting point	**200.00 °C**	**473.15 K**			
CSID	258050	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	430.5618	**H bond donors**	0	**ACD/LogP**	9.13
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.19 g/cm^3
SMILES	o1c5c(nc1c2sc(cc2)c3nc4cc(ccc4o3)C(C)(C)C)cc(cc5)C(C)(C)C				
STD InChIKey	AIXZBGVLNVRQSS-UHFFFAOYAN				

Melting Points

mp °C	source
201.00	Alfa Aesar
199.00	Oxford University MSDS

2,5-di-t-butylbenzene-1,4-diol C14H22O2[3, 61, 64]



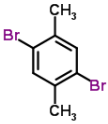
Compound Data

Melting point	**217.33 °C**	**490.48 K**			
CSID	2283	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	222.3233	**H bond donors**	2	**ACD/LogP**	4.02
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.01 g/cm^3
SMILES	Oc1cc(c(O)cc1C(C)(C)C)C(C)(C)C				
STD InChIKey	JZODKRWQWUWGCD-UHFFFAOYAA				

Melting Points

mp °C	source
216.00	Alfa Aesar
218.00	Oxford University MSDS
218.00	PHYSPROP

2,5-dibromo-p-xylene C8H8Br2[3, 48]



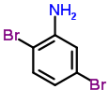
Compound Data

Melting point	**73.50 °C**	**346.65 K**			
CSID	59562	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	263.9571	**H bond donors**	0	**ACD/LogP**	4.71
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.71 g/cm^3
SMILES	Brc1c(cc(Br)c(c1)C)C				
STD InChIKey	QENIALCDPFDFHX-UHFFFAOYAM				

Melting Points

mp °C	source
73.00	Alfa Aesar
74.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2,5-dibromoaniline C6H5Br2N[2, 3]



Compound Data

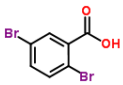
Melting point	**52.50 °C**	**325.65 K**			
CSID	69628	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	250.9186	**H bond donors**	2	**ACD/LogP**	3.38
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.02 g/cm^3
SMILES	Brc1ccc(Br)c(N)c1				
STD InChIKey	WRTAZRGRFBCKBU-UHFFFAOYAR				

Melting Points

mp °C	source
51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar

2,5-dibromobenzoic acid C7H4Br2O2[3, 64]

Compound Data



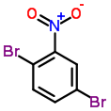
Melting point	**156.00 °C**	**429.15 K**			
CSID	11398	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	279.9135	**H bond donors**	1	**ACD/LogP**	3.63
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.08 g/cm^3
SMILES	c1cc(c(cc1Br)C(=O)O)Br				
STD InChIKey	SQQKOTVDGCJJKI-UHFFFAOYAU				

Melting Points

mp °C	source
155.00	Alfa Aesar
157.00	PHYSPROP

2,5-dibromonitrobenzene C6H3Br2NO2[2, 3, 64]

Compound Data



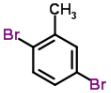
Melting point	**83.83 °C**	**356.98 K**			
CSID	69450	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	280.9015	**H bond donors**	0	**ACD/LogP**	3.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.10 g/cm^3
SMILES	O=[N+]([O-])c1cc(Br)ccc1Br				
STD InChIKey	WRGKKASJBOREMB-UHFFFAOYAM				

Melting Points

mp °C	source
82.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
84.00	Alfa Aesar
85.50	PHYSPROP

2,5-dibromotoluene C7H6Br2[2, 3, 64]

Compound Data



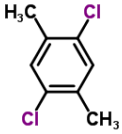
Melting point	**5.53 °C**	**278.68 K**			
CSID	11511	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	249.9305	**H bond donors**	0	**ACD/LogP**	4.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.81 g/cm^3
SMILES	Brc1ccc(Br)c(c1)C				
STD InChIKey	QKEZTJYRBHOKHH-UHFFFAOYAR				

Melting Points

mp °C	source
5.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
6.00	Alfa Aesar
5.60	PHYSPROP

2,5-dichloro-1,4-dimethylbenzene C8H8Cl2[3, 31, 48, 64]

Compound Data



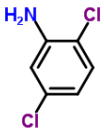
Melting point	**69.50 °C**	**342.65 K**			
CSID	13868642	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	175.0551	**H bond donors**	0	**ACD/LogP**	4.26
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	Clc1cc(C)c(Cl)cc1C				
STD InChIKey	UTGSRNVBAFCOEU-UHFFFAOYAL				

Melting Points

mp °C	source
69.00	Alfa Aesar
68.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
70.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
71.00	PHYSPROP

2,5-dichloroaniline C6H5Cl2N[2, 3, 61, 64]

Compound Data



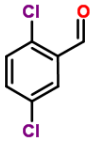
Melting point	**49.50 °C**	**322.65 K**			
CSID	13869655	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.0166	**H bond donors**	2	**ACD/LogP**	2.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Clc1ccc(Cl)c(N)c1				
STD InChIKey	AVYGCQXNNJPXSS-UHFFFAOYAK				

Melting Points

mp °C	source
50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
50.00	Alfa Aesar
48.00	Oxford University MSDS
50.00	PHYSPROP

2,5-dichlorobenzaldehyde C7H4Cl2O[3, 64]

Compound Data



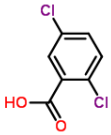
Melting point	**57.00 °C**	**330.15 K**			
CSID	21111840	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.0121	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	O=Cc1cc(Cl)ccc1Cl				
STD InChIKey	BUXHYMZMVMNDMG-UHFFFAOYAM				

Melting Points

mp °C	source
56.00	Alfa Aesar
58.00	PHYSPROP

2,5-dichlorobenzoic acid C7H4Cl2O2[2, 3, 61, 64]

Compound Data



Melting point	**153.97 °C**	**427.12 K**			
CSID	10801689	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	191.0115	**H bond donors**	1	**ACD/LogP**	2.97
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	O=C(O)c1cc(Cl)ccc1Cl				
STD InChIKey	QVTQYSFCFOGITD-UHFFFAOYAT				

Melting Points

mp °C	source
156.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
153.00	Alfa Aesar
152.50	Oxford University MSDS
154.40	PHYSPROP

2,5-dichloronitrobenzene C6H3Cl2NO2[2, 3, 64]

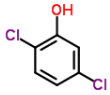
Compound Data

Melting point	**55.67 °C**	**328.82 K**			
CSID	21111865	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.9995	**H bond donors**	0	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3
SMILES	O=[N+]([O-])c1cc(Cl)ccc1Cl				
STD InChIKey	RZKKOBGFCAHLCZ-UHFFFAOYAY				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
56.00	PHYSPROP

2,5-dichlorophenol C6H4Cl2O[2, 3, 64]



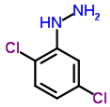
Compound Data

Melting point	**57.67 °C**	**330.82 K**			
CSID	65	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.0014	**H bond donors**	1	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	Clc1ccc(Cl)c(O)c1				
STD InChIKey	RANCECPPZPIPNO-UHFFFAOYAZ				

Melting Points

mp °C	source
57.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
57.00	Alfa Aesar
59.00	PHYSPROP

2,5-dichlorophenylhydrazine C6H6Cl2N2[3, 64]



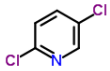
Compound Data

Melting point	**103.25 °C**	**376.40 K**			
CSID	8998	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	177.0312	**H bond donors**	3	**ACD/LogP**	2.72
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.48 g/cm^3
SMILES	Clc1ccc(Cl)cc1NN				
STD InChIKey	LZKWWERBNXLGLI-UHFFFAOYAL				

Melting Points

mp °C	source
104.00	Alfa Aesar
102.50	PHYSPROP

2,5-dichloropyridine C5H3Cl2N[3, 64]



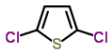
Compound Data

Melting point	**60.75 °C**	**333.90 K**			
CSID	25757	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	147.99	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	c1cc(ncc1Cl)Cl				
STD InChIKey	GCTFDMFLLBCLPF-UHFFFAOYAP				

Melting Points

mp °C	source
61.00	Alfa Aesar
60.50	PHYSPROP

2,5-dichlorothiophene C4H2Cl2S[3, 64]



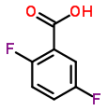
Compound Data

Melting point	**-40.75 °C**	**232.40 K**			
CSID	17474	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	153.0297	**H bond donors**	0	**ACD/LogP**	3.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	Clc1sc(Cl)cc1				
STD InChIKey	FGYBDASKYMSNCX-UHFFFAOYAS				

Melting Points

mp °C	source
-41.00	Alfa Aesar
-40.50	PHYSPROP

2,5-difluorobenzoic acid C7H4F2O2[3, 64]



Compound Data

Melting point	**131.50 °C**	**404.65 K**			
CSID	68816	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1023	**H bond donors**	1	**ACD/LogP**	2.19
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	O=C(O)c1cc(F)ccc1F				
STD InChIKey	LBQMIAVIGLLBGW-UHFFFAOYAH				

Melting Points

mp °C	source
130.00	Alfa Aesar
133.00	PHYSPROP

2,5-dihydrothiophene 1,1-dioxide C4H6O2S[3, 61, 64]

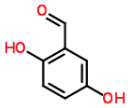
Compound Data

Melting point	**64.67 °C**	**337.82 K**			
CSID	6253	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1542	**H bond donors**	0	**ACD/LogP**	-0.87
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.33 g/cm^3
SMILES	O=S1(=O)C/C=C\C1				
STD InChIKey	MBDNRNMVTZADMQ-UHFFFAOYAO				

Melting Points

mp °C	source
65.00	Alfa Aesar
64.50	Oxford University MSDS
64.50	PHYSPROP

2,5-dihydroxybenzaldehyde C7H6O3[2, 3]



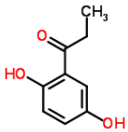
Compound Data

Melting point	**98.50 °C**	**371.65 K**			
CSID	64111	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	138.1207	**H bond donors**	2	**ACD/LogP**	1.12
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.41 g/cm^3
SMILES	O=Cc1cc(O)ccc1O				
STD InChIKey	CLFRCXCBWIQVRN-UHFFFAOYAT				

Melting Points

mp °C	source
98.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
99.00	Alfa Aesar

2,5-dihydroxypropiophenone C9H10O3[3, 64]



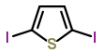
Compound Data

Melting point	**97.25 °C**	**370.40 K**			
CSID	63495	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	2	**ACD/LogP**	2.12
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.24 g/cm^3
SMILES	O=C(c1cc(O)ccc1O)CC				
STD InChIKey	CFQYIIXIHXUPQT-UHFFFAOYAB				

Melting Points

mp °C	source
98.00	Alfa Aesar
96.50	PHYSPROP

2,5-diiodothiophene C4H2I2S[3, 64]



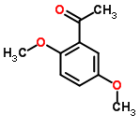
Compound Data

Melting point	**41.25 °C**	**314.40 K**			
CSID	62577	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	335.9326	**H bond donors**	0	**ACD/LogP**	3.50
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.73 g/cm^3
SMILES	Ic1sc(I)cc1				
STD InChIKey	PNYWRAHWEIOAGK-UHFFFAOYAR				

Melting Points

mp °C	source
41.00	Alfa Aesar
41.50	PHYSPROP

2,5-dimethoxyacetophenone C10H12O3[2, 3]



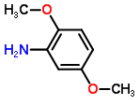
Compound Data

Melting point	**19.50 °C**	**292.65 K**			
CSID	64152	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	0	**ACD/LogP**	2.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	O=C(c1cc(OC)ccc1OC)C				
STD InChIKey	FAXUIYJKGGUCBO-UHFFFAOYAT				

Melting Points

mp °C	source
20.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
19.00	Alfa Aesar

2,5-dimethoxyaniline C8H11NO2[3, 64]



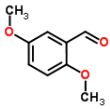
Compound Data

Melting point	**81.25 °C**	**354.40 K**			
CSID	13869661	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	153.1784	**H bond donors**	2	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	COc1ccc(c(c1)N)OC				
STD InChIKey	NAZDVUBIEPVUKE-UHFFFAOYAY				

Melting Points

mp °C	source
80.00	Alfa Aesar
82.50	PHYSPROP

2,5-dimethoxybenzaldehyde C9H10O3[2, 3, 64]



Compound Data

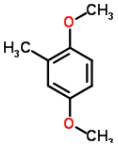
Melting point	**51.00 °C**	**324.15 K**			
CSID	60092	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	0	**ACD/LogP**	1.86
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	COc1ccc(c(c1)C=O)OC				
STD InChIKey	AFUKNJHPZAVHGQ-UHFFFAOYAN				

Melting Points

mp °C	source
52.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
49.00	Alfa Aesar
52.00	PHYSPROP

2,5-dimethoxytoluene C9H12O2[3, 7]

Compound Data



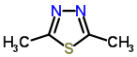
Melting point	**17.50 °C**	**290.65 K**			
CSID	81759	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	152.1904	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	O(c1ccc(OC)cc1C)C				
STD InChIKey	IQISOVKPFBLQIQ-UHFFFAOYAE				

Melting Points

mp °C	source
20.00	Alfa Aesar
15.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

2,5-dimethyl-1,3,4-thiadiazole C4H6N2S[3, 64]

Compound Data



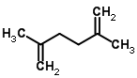
Melting point	**64.00 °C**	**337.15 K**			
CSID	87514	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.1688	**H bond donors**	0	**ACD/LogP**	0.03
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.17 g/cm^3
SMILES	n1nc(sc1C)C				
STD InChIKey	JXQGICFGPUAVLJ-UHFFFAOYAM				

Melting Points

mp °C	source
63.00	Alfa Aesar
65.00	PHYSPROP

2,5-dimethyl-1,5-hexadiene C8H14[3, 64]

Compound Data



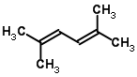
Melting point	**-75.30 °C**	**197.85 K**			
CSID	11818	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	3.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.73 g/cm^3
SMILES	C=C(/C)CCC(=C)\C				
STD InChIKey	DSAYAFZWRDYBQY-UHFFFAOYAP				

Melting Points

mp °C	source
-75.00	Alfa Aesar
-75.60	PHYSPROP

2,5-dimethyl-2,4-hexadiene C8H14[2, 3]

Compound Data



Melting point	**12.50 °C**	**285.65 K**			
CSID	12451	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	4.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.75 g/cm^3
SMILES	C(=C\C=C(/C)C)(\C)C				
STD InChIKey	DZPCYXCBXGQBRN-UHFFFAOYAU				

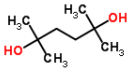
Melting Points

mp °C	source
13.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
12.00	Alfa Aesar

2,5-dimethyl-2,5-hexanediol C8H18O2[3, 64]

Compound Data

Melting point	**90.50 °C**	**363.65 K**			
CSID	7740	**H bond acceptors**	2	**Rule of 5 violations**	0



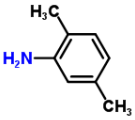
Molecular weight	146.2273	**H bond donors**	2	**ACD/LogP**	0.37
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	0.94 g/cm^3
SMILES	OC(C)(CCC(O)(C)C)C				
STD InChIKey	ZWNMRZQYWRLGMM-UHFFFAOYAJ				

Melting Points

mp °C	source
89.00	Alfa Aesar
92.00	PHYSPROP

2,5-dimethylaniline C8H11N[2, 3, 32, 64]

Compound Data



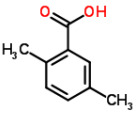
Melting point	**14.50 °C**	**287.65 K**			
CSID	13869434	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	Cc1cc(N)c(C)cc1				
STD InChIKey	VOWZNBNDMFLQGM-UHFFFAOYAX				

Melting Points

mp °C	source
12.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
15.00	Alfa Aesar
15.50	DrugBank
15.50	PHYSPROP

2,5-dimethylbenzoic acid C9H10O2[3, 48, 64]

Compound Data



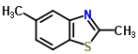
Melting point	**133.33 °C**	**406.48 K**			
CSID	11399	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	2.81
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	O=C(O)c1cc(ccc1C)C				
STD InChIKey	XZRHNAFEYMSXRG-UHFFFAOYAD				

Melting Points

mp °C	source
134.00	Alfa Aesar
134.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
132.00	PHYSPROP

2,5-dimethylbenzothiazole C9H9NS[3, 64]

Compound Data

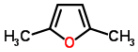


Melting point	**39.00 °C**	**312.15 K**			
CSID	6957	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.2395	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.18 g/cm^3
SMILES	n1c2cc(ccc2sc1C)C				
STD InChIKey	XHANCLXYCNTZMM-UHFFFAOYAT				

Melting Points

mp °C	source
40.00	Alfa Aesar
38.00	PHYSPROP

2,5-dimethylfuran C6H8O[3, 64]



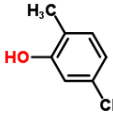
Compound Data

Melting point	**-62.40 °C**	**210.75 K**			
CSID	11763	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	96.1271	**H bond donors**	0	**ACD/LogP**	1.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.92 g/cm^3
SMILES	Cc1ccc(o1)C				
STD InChIKey	GSNUFIFRDBKVIE-UHFFFAOYAS				

Melting Points

mp °C	source
-62.00	Alfa Aesar
-62.80	PHYSPROP

2,5-dimethylphenol C8H10O[3, 28, 31, 64, 72]



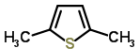
Compound Data

Melting point	**75.12 °C**	**348.27 K**			
CSID	13839128	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	Cc1cc(O)c(C)cc1				
STD InChIKey	NKTOLZVEWDHZMU-UHFFFAOYAH				

Melting Points

mp °C	source
76.00	Alfa Aesar
74.80	CRC Handbook of Chemistry and Physics
74.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
74.80	PHYSPROP
76.00	Sigma-Aldrich

2,5-dimethylthiophene C6H8S[3, 64]



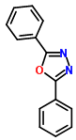
Compound Data

Melting point	**-62.80 °C**	**210.35 K**			
CSID	11998	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.1927	**H bond donors**	0	**ACD/LogP**	2.82
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.01 g/cm^3
SMILES	s1c(ccc1C)C				
STD InChIKey	GWQOOADXMVQEFT-UHFFFAOYAY				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-62.60	PHYSPROP

2,5-diphenyl-1,3,4-oxadiazole C14H10N2O[3, 64]



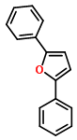
Compound Data

Melting point	**139.50 °C**	**412.65 K**			
CSID	12355	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	222.242	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	n1nc(oc1c2ccccc2)c3ccccc3				
STD InChIKey	DCJKUXYSYJBBRD-UHFFFAOYAH				

Melting Points

mp °C	source
140.00	Alfa Aesar
139.00	PHYSPROP

2,5-diphenylfuran C16H12O[3, 64]



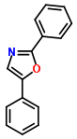
Compound Data

Melting point	**89.50 °C**	**362.65 K**			
CSID	63567	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	220.2659	**H bond donors**	0	**ACD/LogP**	5.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	o1c(ccc1c2ccccc2)c3ccccc3				
STD InChIKey	VUPDHIIPAKIKAB-UHFFFAOYAN				

Melting Points

mp °C	source
88.00	Alfa Aesar
91.00	PHYSPROP

2,5-diphenyloxazole C15H11NO[3, 64]



Compound Data

Melting point	**73.00 °C**	**346.15 K**			
CSID	6838	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	221.2539	**H bond donors**	0	**ACD/LogP**	4.12
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.13 g/cm^3
SMILES	n1cc(oc1c2ccccc2)c3ccccc3				
STD InChIKey	CNRNYORZJGVOSY-UHFFFAOYAG				

Melting Points

mp °C	source
72.00	Alfa Aesar
74.00	PHYSPROP

2,5-norbornadiene C7H8[3, 64]

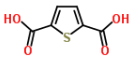
Compound Data

Melting point	**-19.55 °C**	**253.60 K**			
CSID	8160	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	92.1384	**H bond donors**	0	**ACD/LogP**	2.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	C\1=C\C2/C=C\C/1C2				
STD InChIKey	SJYNFBVQFBRSIB-UHFFFAOYAK				

Melting Points

mp °C	source
-20.00	Alfa Aesar
-19.10	PHYSPROP

2,5-thiophenedicarboxylic acid C6H4O4S[3, 64]



Compound Data

Melting point	**358.50 °C**	**631.65 K**			
CSID	19099	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.1586	**H bond donors**	2	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.66 g/cm^3
SMILES	O=C(O)c1sc(C(=O)O)cc1				
STD InChIKey	YCGAZNXXGKTASZ-UHFFFAOYAF				

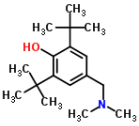
Melting Points

mp °C	source
358.00	Alfa Aesar
359.00	PHYSPROP

2,6-di-t-butyl-4-(dimethylaminomethyl)phenol C17H29NO[3, 64]

Compound Data

Melting point	**92.25 °C**	**365.40 K**



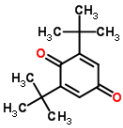
CSID	59976	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	263.4183	**H bond donors**	1	**ACD/LogP**	4.62
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	0.95 g/cm^3
SMILES	Oc1c(cc(cc1C(C)(C)C)CN(C)C)C(C)(C)C				
STD InChIKey	VMZVBRIIHDRYGK-UHFFFAOYAR				

Melting Points

mp °C	source
91.00	Alfa Aesar
93.50	PHYSPROP

2,6-di-t-butylbenzoquinone C14H20O2[3, 64]

Compound Data



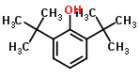
Melting point	**66.50 °C**	**339.65 K**			
CSID	12336	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	220.3074	**H bond donors**	0	**ACD/LogP**	3.90
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	O=C/1/C(=C\C(=O)\C=C\1C(C)(C)C)C(C)(C)C				
STD InChIKey	RDQSIADLBQFVMY-UHFFFAOYAS				

Melting Points

mp °C	source
67.00	Alfa Aesar
66.00	PHYSPROP

2,6-di-t-butylphenol C14H22O[3, 61, 64]

Compound Data



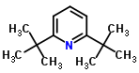
Melting point	**37.50 °C**	**310.65 K**			
CSID	29135	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	206.3239	**H bond donors**	1	**ACD/LogP**	4.86
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.93 g/cm^3
SMILES	Oc1c(cccc1C(C)(C)C)C(C)(C)C				
STD InChIKey	DKCPKDPYUFEZCP-UHFFFAOYAK				

Melting Points

mp °C	source
37.00	Alfa Aesar
36.50	Oxford University MSDS
39.00	PHYSPROP

2,6-di-t-butylpyridine C13H21N[61, 64]

Compound Data



Melting point	**2.10 °C**	**275.25 K**			
CSID	61785	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	191.3125	**H bond donors**	0	**ACD/LogP**	4.10
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.89 g/cm^3
SMILES	n1c(cccc1C(C)(C)C)C(C)(C)C				
STD InChIKey	UWKQJZCTQGMHKD-UHFFFAOYAA				

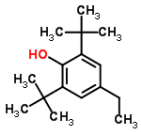
Melting Points

mp °C	source
2.00	Oxford University MSDS
2.20	PHYSPROP

2,6-di-tert-butyl-4-ethylphenol C16H26O[3, 64]

Compound Data

Melting point	**43.50 °C**	**316.65 K**



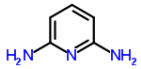
CSID	18924	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	234.377	**H bond donors**	1	**ACD/LogP**	5.85
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.92 g/cm^3
SMILES	Oc1c(cc(cc1C(C)(C)C)CC)C(C)(C)C				
STD InChIKey	BVUXDWXKPROUDO-UHFFFAOYAH				

Melting Points

mp °C	source
43.00	Alfa Aesar
44.00	PHYSPROP

2,6-diaminopyridine C5H7N3[3, 35, 64]

Compound Data



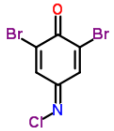
Melting point	**121.00 °C**	**394.15 K**			
CSID	8528	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	109.1292	**H bond donors**	4	**ACD/LogP**	0.55
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	c1cc(nc(c1)N)N				
STD InChIKey	VHNQIURBCCNWDN-UHFFFAOYAB				

Melting Points

mp °C	source
120.00	Alfa Aesar
121.50	EPISuite-ChemSpider
121.50	PHYSPROP

2,6-dibromo-N-chloroquinonimine C6H2Br2ClNO[3, 64]

Compound Data



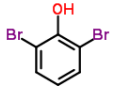
Melting point	**81.50 °C**	**354.65 K**			
CSID	10378	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	299.3472	**H bond donors**	0	**ACD/LogP**	1.97
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.18 g/cm^3
SMILES	Br\C1=CC(=N\Cl)/C=C(/Br)C1=O				
STD InChIKey	JYWKEVKEKOTYEX-UHFFFAOYAP				

Melting Points

mp °C	source
80.00	Alfa Aesar
83.00	PHYSPROP

2,6-dibromophenol C6H4Br2O[3, 64]

Compound Data



Melting point	**55.75 °C**	**328.90 K**			
CSID	11354	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	251.9034	**H bond donors**	1	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.10 g/cm^3
SMILES	c1cc(c(c(c1)Br)O)Br				
STD InChIKey	SSIZLKDLDKIHEV-UHFFFAOYAG				

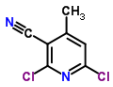
Melting Points

mp °C	source
55.00	Alfa Aesar
56.50	PHYSPROP

2,6-dichloro-3-cyano-4-methylpyridine C7H4Cl2N2[3, 48]

Compound Data

Melting point	**111.50 °C**	**384.65 K**



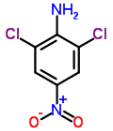
CSID	63319	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	187.0261	**H bond donors**	0	**ACD/LogP**	2.23
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	N#Cc1c(cc(Cl)nc1Cl)C				
STD InChIKey	LSPMHHJCDSFAAY-UHFFFAOYAA				

Melting Points

mp °C	source
110.00	Alfa Aesar
113.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2,6-dichloro-4-nitroaniline C6H4Cl2N2O2[3, 64]

Compound Data



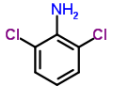
Melting point	**190.00 °C**	**463.15 K**			
CSID	7152	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	207.0142	**H bond donors**	2	**ACD/LogP**	3.54
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.62 g/cm^3
SMILES	Clc1cc(cc(Cl)c1N)[N+]([O-])=O				
STD InChIKey	BIXZHMJUSMUDOQ-UHFFFAOYAH				

Melting Points

mp °C	source
189.00	Alfa Aesar
191.00	PHYSPROP

2,6-dichloroaniline C6H5Cl2N[2, 3, 64]

Compound Data



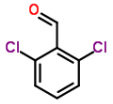
Melting point	**39.33 °C**	**312.48 K**			
CSID	11353	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.0166	**H bond donors**	2	**ACD/LogP**	2.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Clc1cccc(Cl)c1N				
STD InChIKey	JDMFXJULNGEPOI-UHFFFAOYAF				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
39.00	Alfa Aesar
39.00	PHYSPROP

2,6-dichlorobenzaldehyde C7H4Cl2O[2, 3, 35, 61, 64]

Compound Data

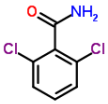


Melting point	**71.10 °C**	**344.25 K**			
CSID	6481	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.0121	**H bond donors**	0	**ACD/LogP**	3.03
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	O=Cc1c(Cl)cccc1Cl				
STD InChIKey	DMIYKWPEFRFTPY-UHFFFAOYAO				

Melting Points

mp °C	source
71.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
71.00	Alfa Aesar
71.50	EPISuite-ChemSpider
70.50	Oxford University MSDS
71.50	PHYSPROP

2,6-dichlorobenzamide C7H5Cl2NO[2, 3, 64]



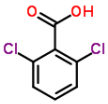
Compound Data

Melting point	**198.17 °C**	**471.32 K**			
CSID	15359	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	190.0267	**H bond donors**	2	**ACD/LogP**	1.13
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.44 g/cm^3
SMILES	O=C(c1c(Cl)cccc1Cl)N				
STD InChIKey	JHSPCUHPSIUQRB-UHFFFAOYAS				

Melting Points

mp °C	source
198.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
199.00	Alfa Aesar
197.50	PHYSPROP

2,6-dichlorobenzoic acid C7H4Cl2O2[2, 3, 61, 64]



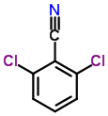
Compound Data

Melting point	**143.75 °C**	**416.90 K**			
CSID	5555	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	191.0115	**H bond donors**	1	**ACD/LogP**	2.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	O=C(O)c1c(Cl)cccc1Cl				
STD InChIKey	MRUDNSFOFOQZDA-UHFFFAOYAC				

Melting Points

mp °C	source
144.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
143.00	Alfa Aesar
144.00	Oxford University MSDS
144.00	PHYSPROP

2,6-dichlorobenzonitrile C7H3Cl2N[2, 3, 61, 64]



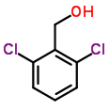
Compound Data

Melting point	**144.12 °C**	**417.27 K**			
CSID	2923	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	172.0114	**H bond donors**	0	**ACD/LogP**	2.79
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	N#Cc1c(Cl)cccc1Cl				
STD InChIKey	YOYAIZYFCNQIRF-UHFFFAOYAG				

Melting Points

mp °C	source
143.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
145.00	Alfa Aesar
144.00	Oxford University MSDS
144.50	PHYSPROP

2,6-dichlorobenzyl alcohol C7H6Cl2O[3, 64]



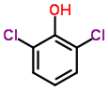
Compound Data

Melting point	**97.50 °C**	**370.65 K**			
CSID	25276	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	1	**ACD/LogP**	2.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	Clc1cccc(Cl)c1CO				
STD InChIKey	WKKHCCZLKYKUDN-UHFFFAOYAY				

Melting Points

mp °C	source
97.00	Alfa Aesar
98.00	PHYSPROP

2,6-dichlorophenol $C_6H_4Cl_2O$[2, 3, 28, 56, 61, 64, 72]



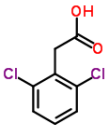
Compound Data

Melting point	**67.07 °C**	**340.22 K**			
CSID	6633	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.0014	**H bond donors**	1	**ACD/LogP**	2.61
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	Clc1cccc(Cl)c1O				
STD InChIKey	HOLHYSJJBXSLMV-UHFFFAOYAE				

Melting Points

mp °C	source
67.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
67.00	Alfa Aesar
68.50	CRC Handbook of Chemistry and Physics
65.00	Merck Index
68.50	Oxford University MSDS
68.50	PHYSPROP
65.00	Sigma-Aldrich

2,6-dichlorophenylacetic acid $C_8H_6Cl_2O_2$[3, 3]



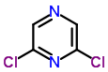
Compound Data

Melting point	**159.50 °C**	**432.65 K**			
CSID	73131	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	205.038	**H bond donors**	1	**ACD/LogP**	2.71
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.46 g/cm^3
SMILES	Clc1cccc(Cl)c1CC(=O)O				
STD InChIKey	SFAILOOQFZNOAU-UHFFFAOYAK				

Melting Points

mp °C	source
159.00	Alfa Aesar
160.00	Alfa Aesar

2,6-dichloropyrazine $C_4H_2Cl_2N_2$[3, 64]



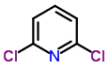
Compound Data

Melting point	**55.25 °C**	**328.40 K**			
CSID	70868	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	148.9781	**H bond donors**	0	**ACD/LogP**	1.48
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	c1c(nc(cn1)Cl)Cl				
STD InChIKey	LSEAAPGIZCDEEH-UHFFFAOYAG				

Melting Points

mp °C	source
54.00	Alfa Aesar
56.50	PHYSPROP

2,6-dichloropyridine $C_5H_3Cl_2N$[3, 64]



Compound Data

Melting point	**87.00 °C**	**360.15 K**			
CSID	16095	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	147.99	**H bond donors**	0	**ACD/LogP**	2.08
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	Clc1nc(Cl)ccc1				
STD InChIKey	FILKGCRCWDMBKA-UHFFFAOYAA				

Melting Points

mp °C	source
86.00	Alfa Aesar
88.00	PHYSPROP

2,6-dichlorothiobenzamide C7H5Cl2NS[3, 64]

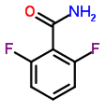
Compound Data

Melting point	**151.25 °C**	**424.40 K**			
CSID	2016563	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	206.0923	**H bond donors**	2	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.47 g/cm^3
SMILES	S=C(c1c(Cl)cccc1Cl)N				
STD InChIKey	KGKGSIUWJCAFPX-UHFFFAOYAZ				

Melting Points

mp °C	source
151.00	Alfa Aesar
151.50	PHYSPROP

2,6-difluorobenzamide C7H5F2NO[3, 64]



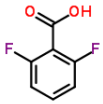
Compound Data

Melting point	**146.75 °C**	**419.90 K**			
CSID	78873	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	157.1175	**H bond donors**	2	**ACD/LogP**	0.58
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	O=C(c1c(F)cccc1F)N				
STD InChIKey	AVRQBXVUUXHRMY-UHFFFAOYAV				

Melting Points

mp °C	source
147.00	Alfa Aesar
146.50	PHYSPROP

2,6-difluorobenzoic acid C7H4F2O2[3, 64]



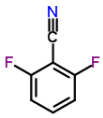
Compound Data

Melting point	**158.50 °C**	**431.65 K**			
CSID	9413	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1023	**H bond donors**	1	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	O=C(O)c1c(F)cccc1F				
STD InChIKey	ONOTYLMNTZNAQZ-UHFFFAOYAX				

Melting Points

mp °C	source
158.00	Alfa Aesar
159.00	PHYSPROP

2,6-difluorobenzonitrile C7H3F2N[3, 64]



Compound Data

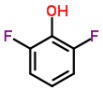
Melting point	**30.50 °C**	**303.65 K**			
CSID	67268	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	139.1022	**H bond donors**	0	**ACD/LogP**	1.40
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	N#Cc1c(F)cccc1F				
STD InChIKey	BNBRIFIJRKJGEI-UHFFFAOYAP				

Melting Points

mp °C	source
30.00	Alfa Aesar

31.00	PHYSPROP

2,6-difluorophenol C6H4F2O[3, 64]



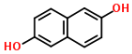
Compound Data

Melting point	**38.75 °C**	**311.90 K**			
CSID	85185	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	130.0922	**H bond donors**	1	**ACD/LogP**	1.98
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	Fc1cccc(F)c1O				
STD InChIKey	CKKOVFGIBXCEIJ-UHFFFAOYAW				

Melting Points

mp °C	source
38.00	Alfa Aesar
39.50	PHYSPROP

2,6-dihydroxynaphthalene C10H8O2[3, 64]



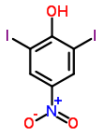
Compound Data

Melting point	**222.00 °C**	**495.15 K**			
CSID	84452	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.1693	**H bond donors**	2	**ACD/LogP**	1.90
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	Oc1ccc2c(c1)ccc(O)c2				
STD InChIKey	MNZMMCVIXORAQL-UHFFFAOYAZ				

Melting Points

mp °C	source
224.00	Alfa Aesar
220.00	PHYSPROP

2,6-diiodo-4-nitrophenol C6H3I2NO3[3, 61, 64]



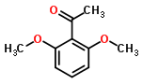
Compound Data

Melting point	**155.67 °C**	**428.82 K**			
CSID	9002	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	390.9019	**H bond donors**	1	**ACD/LogP**	3.37
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.72 g/cm^3
SMILES	Ic1cc([N+](=O)[O-])cc(I)c1O				
STD InChIKey	UVGTXNPVQOQFQW-UHFFFAOYAA				

Melting Points

mp °C	source
153.00	Alfa Aesar
157.00	Oxford University MSDS
157.00	PHYSPROP

2,6-dimethoxyacetophenone C10H12O3[3, 64]



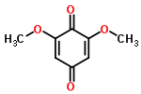
Compound Data

Melting point	**69.50 °C**	**342.65 K**			
CSID	15435	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	0	**ACD/LogP**	1.98
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	O=C(c1c(OC)cccc1OC)C				
STD InChIKey	XEUGKOFTNAYMMX-UHFFFAOYAM				

Melting Points

mp °C	source
70.00	Alfa Aesar
69.00	PHYSPROP

2,6-dimethoxybenzoquinone C8H8O4[3, 61, 64]



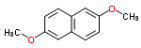
Compound Data

Melting point	**254.67 °C**	**527.82 K**			
CSID	61560	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	0	**ACD/LogP**	0.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	O=C1C(/OC)=C\C(=O)\C=C1\OC				
STD InChIKey	OLBNOBQOQZRLMP-UHFFFAOYAL				

Melting Points

mp °C	source
255.00	Alfa Aesar
253.00	Oxford University MSDS
256.00	PHYSPROP

2,6-dimethoxynaphthalene C12H12O2[3, 48]



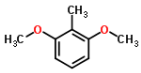
Compound Data

Melting point	**151.50 °C**	**424.65 K**			
CSID	71934	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	188.2225	**H bond donors**	0	**ACD/LogP**	3.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.10 g/cm^3
SMILES	O(c1ccc2c(c1)ccc(OC)c2)C				
STD InChIKey	AHKDVDYNDXGFPP-UHFFFAOYAF				

Melting Points

mp °C	source
153.00	Alfa Aesar
150.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

2,6-dimethoxytoluene C9H12O2[2, 3, 64]



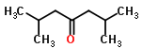
Compound Data

Melting point	**39.67 °C**	**312.82 K**			
CSID	72054	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	152.1904	**H bond donors**	0	**ACD/LogP**	2.39
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	O(c1cccc(OC)c1C)C				
STD InChIKey	FPEUDBGJAVKAEE-UHFFFAOYAX				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
39.00	Alfa Aesar
40.00	PHYSPROP

2,6-dimethyl-4-heptanone C9H18O[3, 64]



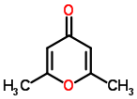
Compound Data

Melting point	**-41.75 °C**	**231.40 K**			
CSID	7670	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	142.2386	**H bond donors**	0	**ACD/LogP**	2.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.81 g/cm^3
SMILES	O=C(CC(C)C)CC(C)C				
STD InChIKey	PTTPXKJBFFKCEK-UHFFFAOYAW				

Melting Points

mp °C	source
-42.00	Alfa Aesar
-41.50	PHYSPROP

2,6-dimethyl-4-pyrone C7H8O2[3, 64]



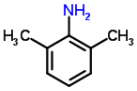
Compound Data

Melting point	**133.00 °C**	**406.15 K**			
CSID	13262	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	0	**ACD/LogP**	0.10
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.06 g/cm^3
SMILES	O=C\1/C=C(\O/C(=C/1)C)C				
STD InChIKey	VSYFZULSKMFUJJ-UHFFFAOYAS				

Melting Points

mp °C	source
134.00	Alfa Aesar
132.00	PHYSPROP

2,6-dimethylaniline C8H11N[2, 3, 61, 64]



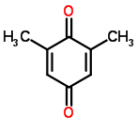
Compound Data

Melting point	**10.55 °C**	**283.70 K**			
CSID	6630	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	Nc1c(cccc1C)C				
STD InChIKey	UFFBMTHBGFGIHF-UHFFFAOYAI				

Melting Points

mp °C	source
12.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
11.00	Alfa Aesar
8.00	Oxford University MSDS
11.20	PHYSPROP

2,6-dimethylbenzoquinone C8H8O2[3, 61, 64]



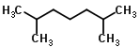
Compound Data

Melting point	**70.83 °C**	**343.98 K**			
CSID	61542	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	0	**ACD/LogP**	1.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	O=C\1\C=C(/C(=O)/C(=C/1)C)C				
STD InChIKey	SENUUPBBLQWHMF-UHFFFAOYAI				

Melting Points

mp °C	source
70.00	Alfa Aesar
70.00	Oxford University MSDS
72.50	PHYSPROP

2,6-dimethylheptane C9H20[4, 64]



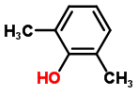
Compound Data

Melting point	**-102.95 °C**	**170.20 K**			
CSID	13450	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	5.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)CCCC(C)C				
STD InChIKey	KBPCCVWUMVGXGF-UHFFFAOYAV				

Melting Points

mp °C	source
-103.00	American Petroleum Institute. Research Project 44; Selected ...
-102.90	PHYSPROP

2,6-dimethylphenol C8H10O[3, 31, 61, 64]



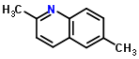
Compound Data

Melting point	**47.42 °C**	**320.57 K**			
CSID	13839174	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	Cc1cccc(C)c1O				
STD InChIKey	NXXYKOUNUYWIHA-UHFFFAOYAM				

Melting Points

mp °C	source
46.00	Alfa Aesar
49.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
49.00	Oxford University MSDS
45.70	PHYSPROP

2,6-dimethylquinoline C11H11N[3, 64]



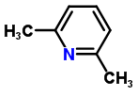
Compound Data

Melting point	**58.50 °C**	**331.65 K**			
CSID	12840	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	157.2117	**H bond donors**	0	**ACD/LogP**	3.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	n1c(ccc2cc(ccc12)C)C				
STD InChIKey	JJPSZKIOGBRMHK-UHFFFAOYAO				

Melting Points

mp °C	source
57.00	Alfa Aesar
60.00	PHYSPROP

2,6-lutidine C7H9N[3, 61, 64]



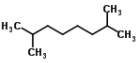
Compound Data

Melting point	**-6.37 °C**	**266.78 K**			
CSID	13842613	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.93 g/cm^3
SMILES	Cc1cccc(C)n1				
STD InChIKey	OISVCGZHLKNMSJ-UHFFFAOYAH				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-6.00	Oxford University MSDS
-6.10	PHYSPROP

2,7-dimethyloctane C10H22[3, 4, 64]



Compound Data

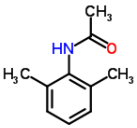
Melting point	**-54.63 °C**	**218.52 K**			
CSID	13451	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.70
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.73 g/cm^3
SMILES	CC(C)CCCCC(C)C				
STD InChIKey	KEVMYFLMMDUPJE-UHFFFAOYAL				

Melting Points

mp °C	source
-55.00	Alfa Aesar

-54.00	American Petroleum Institute. Research Project 44; Selected ...
-54.90	PHYSPROP

2',6'-dimethylacetanilide $C_{10}H_{13}NO$[3, 64]



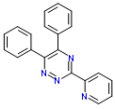
Compound Data

Melting point	**182.00 °C**	**455.15 K**			
CSID	15753	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	163.2163	**H bond donors**	1	**ACD/LogP**	2.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	O=C(Nc1c(cccc1C)C)C				
STD InChIKey	NRPTXWYBRKRZES-UHFFFAOYAQ				

Melting Points

mp °C	source
181.00	Alfa Aesar
183.00	PHYSPROP

3-(2-pyridyl)-5,6-diphenyl-1,2,4-triazine $C_{20}H_{14}N_4$[61, 64]



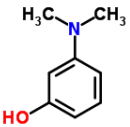
Compound Data

Melting point	**191.50 °C**	**464.65 K**			
CSID	63757	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	310.352	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.20 g/cm^3
SMILES	n2c(nnc(c1ccccc1)c2c3ccccc3)c4ncccc4				
STD InChIKey	OTMYLOBWDNFTLO-UHFFFAOYAF				

Melting Points

mp °C	source
191.00	Oxford University MSDS
192.00	PHYSPROP

3-(dimethylamino)phenol $C_8H_{11}NO$[3, 61, 64]



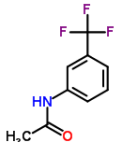
Compound Data

Melting point	**83.67 °C**	**356.82 K**			
CSID	7143	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	137.179	**H bond donors**	1	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	Oc1cccc(N(C)C)c1				
STD InChIKey	MESJRHHDBDCQTH-UHFFFAOYAC				

Melting Points

mp °C	source
82.00	Alfa Aesar
83.00	Oxford University MSDS
86.00	PHYSPROP

3-(trifluoromethyl)acetanilide $C_9H_8F_3NO$[3, 64]



Compound Data

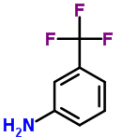
Melting point	**104.75 °C**	**377.90 K**			
CSID	9219	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	203.1611	**H bond donors**	1	**ACD/LogP**	2.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	O=C(Nc1cc(ccc1)C(F)(F)F)C				
STD InChIKey	HNIPNANLYHXYDE-UHFFFAOYAI				

Melting Points

mp °C	source
105.00	Alfa Aesar

104.50	PHYSPROP

3-(trifluoromethyl)aniline C7H6F3N[3, 64]



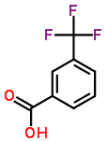
Compound Data

Melting point	**5.75 °C**	**278.90 K**			
CSID	7097	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	161.1244	**H bond donors**	2	**ACD/LogP**	2.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	FC(F)(F)c1cc(N)ccc1				
STD InChIKey	VIUDTWATMPPKEL-UHFFFAOYAM				

Melting Points

mp °C	source
6.00	Alfa Aesar
5.50	PHYSPROP

3-(trifluoromethyl)benzoic acid C8H5F3O2[3, 64]



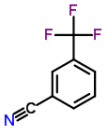
Compound Data

Melting point	**105.25 °C**	**378.40 K**			
CSID	9569	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	190.1193	**H bond donors**	1	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	FC(F)(F)c1cccc(C(=O)O)c1				
STD InChIKey	FQXQBFUUVCDIRK-UHFFFAOYAO				

Melting Points

mp °C	source
105.00	Alfa Aesar
105.50	PHYSPROP

3-(trifluoromethyl)benzonitrile C8H4F3N[3, 64]



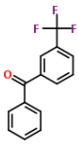
Compound Data

Melting point	**15.25 °C**	**288.40 K**			
CSID	61101	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	171.1193	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	FC(F)(F)c1cccc(C#N)c1				
STD InChIKey	OGOBINRVCUWLGN-UHFFFAOYAZ				

Melting Points

mp °C	source
16.00	Alfa Aesar
14.50	PHYSPROP

3-(trifluoromethyl)benzophenone C14H9F3O[3, 64]



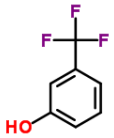
Compound Data

Melting point	**52.25 °C**	**325.40 K**			
CSID	62965	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	250.2159	**H bond donors**	0	**ACD/LogP**	4.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	FC(F)(F)c2cccc(C(=O)c1ccccc1)c2				
STD InChIKey	IOXDAYKKVHAKSX-UHFFFAOYAE				

Melting Points

mp °C	source
52.00	Alfa Aesar
52.50	PHYSPROP

3-(trifluoromethyl)phenol C7H5F3O[3, 64]



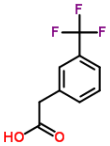
Compound Data

Melting point	**-1.90 °C**	**271.25 K**			
CSID	7098	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.1092	**H bond donors**	1	**ACD/LogP**	2.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	FC(F)(F)c1cc(O)ccc1				
STD InChIKey	UGEJOEBBMPOJMT-UHFFFAOYAP				

Melting Points

mp °C	source
-2.00	Alfa Aesar
-1.80	PHYSPROP

3-(trifluoromethyl)phenylacetic acid C9H7F3O2[3, 64]



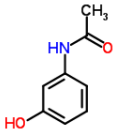
Compound Data

Melting point	**77.50 °C**	**350.65 K**			
CSID	61014	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	204.1459	**H bond donors**	1	**ACD/LogP**	2.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.36 g/cm^3
SMILES	FC(F)(F)c1cccc(c1)CC(=O)O				
STD InChIKey	BLXXCCIBGGBDHI-UHFFFAOYAN				

Melting Points

mp °C	source
78.00	Alfa Aesar
77.00	PHYSPROP

3-acetamidophenol C8H9NO2[2, 3, 64]



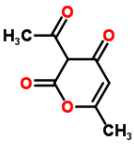
Compound Data

Melting point	**147.00 °C**	**420.15 K**			
CSID	11626	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	0.73
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	O=C(Nc1cccc(O)c1)C				
STD InChIKey	QLNWXBAGRTUKKI-UHFFFAOYAP				

Melting Points

mp °C	source
146.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
148.00	Alfa Aesar
147.00	PHYSPROP

3-acetyl-6-methyl-2-pyranone C8H8O4[3, 64]



Compound Data

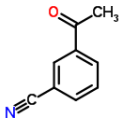
Melting point	**110.00 °C**	**383.15 K**			
CSID	13887609	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	0	**ACD/LogP**	0.35
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	O=C(C)C1C(=O)/C=C(/C)OC1=O				
STD InChIKey	PGRHXDWITVMQBC-UHFFFAOYAH				

Melting Points

mp °C	source
111.00	Alfa Aesar
109.00	PHYSPROP

3-acetylbenzonitrile C9H7NO[3, 7, 64]

Compound Data



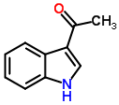
Melting point	**98.67 °C**	**371.82 K**			
CSID	72466	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	145.158	**H bond donors**	0	**ACD/LogP**	1.16
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	N#Cc1cc(C(=O)C)ccc1				
STD InChIKey	SBCFGFDAZCTSRH-UHFFFAOYAN				

Melting Points

mp °C	source
99.00	Alfa Aesar
98.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
99.00	PHYSPROP

3-acetylindole C10H9NO[3, 48, 64]

Compound Data



Melting point	**191.77 °C**	**464.92 K**			
CSID	12275	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	159.1846	**H bond donors**	1	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.19 g/cm^3
SMILES	O=C(c2c1ccccc1nc2)C				
STD InChIKey	VUIMBZIZZFSQEE-UHFFFAOYAP				

Melting Points

mp °C	source
189.00	Alfa Aesar
194.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
192.30	PHYSPROP

3-acetylpyridine C7H7NO[3, 64]

Compound Data

Melting point	**12.75 °C**	**285.90 K**			
CSID	13856009	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	121.1366	**H bond donors**	0	**ACD/LogP**	0.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.06 g/cm^3
SMILES	CC(=O)c1cccnc1				
STD InChIKey	WEGYGNROSJDEIW-UHFFFAOYAV				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.50	PHYSPROP

3-amino-4-chlorobenzoic acid C7H6ClNO2[3, 64]

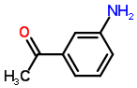
Compound Data

Melting point	**215.00 °C**	**488.15 K**			
CSID	68579	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	3	**ACD/LogP**	1.92
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.48 g/cm^3
SMILES	Clc1ccc(C(=O)O)cc1N				
STD InChIKey	DMGFVJVLVZOSOE-UHFFFAOYAF				

Melting Points

mp °C	source
216.00	Alfa Aesar
214.00	PHYSPROP

3-aminoacetophenone C8H9NO[2, 3, 64]



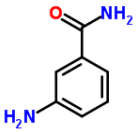
Compound Data

Melting point	**97.17 °C**	**370.32 K**			
CSID	21106518	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	2	**ACD/LogP**	0.69
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.10 g/cm^3
SMILES	O=C(C)c1cc(N)ccc1				
STD InChIKey	CKQHAYFOPRIUOM-UHFFFAOYAX				

Melting Points

mp °C	source
97.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
96.00	Alfa Aesar
98.50	PHYSPROP

3-aminobenzamide C7H8N2O[2, 3, 64]



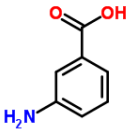
Compound Data

Melting point	**114.50 °C**	**387.65 K**			
CSID	1583	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	136.1512	**H bond donors**	4	**ACD/LogP**	0.33
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C(c1cc(N)ccc1)N				
STD InChIKey	GSCPDZHWVNUUFI-UHFFFAOYAG				

Melting Points

mp °C	source
115.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
113.00	Alfa Aesar
115.50	PHYSPROP

3-aminobenzoic acid C7H7NO2[2, 3, 64]



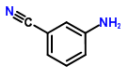
Compound Data

Melting point	**173.67 °C**	**446.82 K**			
CSID	7141	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	3	**ACD/LogP**	0.78
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=C(O)c1cc(N)ccc1				
STD InChIKey	XFDUHJPVQKIXHO-UHFFFAOYAM				

Melting Points

mp °C	source
173.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
175.00	Alfa Aesar
173.00	PHYSPROP

3-aminobenzonitrile C7H6N2[2, 3, 64]



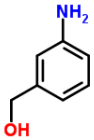
Compound Data

Melting point	**52.77 °C**	**325.92 K**			
CSID	21111842	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1359	**H bond donors**	2	**ACD/LogP**	1.07
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	N#Cc1cc(N)ccc1				
STD InChIKey	NJXPYZHXZZCTNI-UHFFFAOYAM				

Melting Points

mp °C	source
52.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
52.00	Alfa Aesar
54.30	PHYSPROP

3-aminobenzyl alcohol C7H9NO[3, 7]



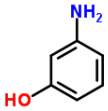
Compound Data

Melting point	**94.00 °C**	**367.15 K**			
CSID	72534	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	123.1525	**H bond donors**	3	**ACD/LogP**	-0.25
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	OCc1cc(N)ccc1				
STD InChIKey	OJZQOQNSUZLSMV-UHFFFAOYAX				

Melting Points

mp °C	source
93.00	Alfa Aesar
95.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

3-aminophenol C6H7NO[2, 3, 61, 64]



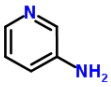
Compound Data

Melting point	**124.25 °C**	**397.40 K**			
CSID	11080	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	3	**ACD/LogP**	0.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	Oc1cccc(N)c1				
STD InChIKey	CWLKGDAVCFYWJK-UHFFFAOYAM				

Melting Points

mp °C	source
125.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
124.00	Alfa Aesar
125.00	Oxford University MSDS
123.00	PHYSPROP

3-aminopyridine C5H6N2[3, 64]



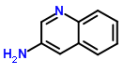
Compound Data

Melting point	**62.75 °C**	**335.90 K**			
CSID	21111768	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.1145	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	Nc1cccnc1				
STD InChIKey	CUYKNJBYIJFRCU-UHFFFAOYAD				

Melting Points

mp °C	source
61.00	Alfa Aesar
64.50	PHYSPROP

3-aminoquinoline C9H8N2[3, 64]



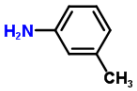
Compound Data

Melting point	**92.75 °C**	**365.90 K**			
CSID	10897	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.1732	**H bond donors**	2	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	n1cc(cc2ccccc12)N				
STD InChIKey	SVNCRRZKBNSMIV-UHFFFAOYAF				

Melting Points

mp °C	source
94.00	Alfa Aesar
91.50	PHYSPROP

3-aminotoluene C7H9N[3, 31, 64]



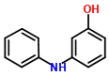
Compound Data

Melting point	**-30.43 °C**	**242.72 K**			
CSID	13860692	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	2	**ACD/LogP**	1.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.99 g/cm^3
SMILES	Cc1cc(N)ccc1				
STD InChIKey	JJYPMNFTHPTTDI-UHFFFAOYAY				

Melting Points

mp °C	source
-30.00	Alfa Aesar
-30.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-31.30	PHYSPROP

3-anilinophenol C12H11NO[3, 61, 64]



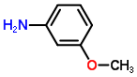
Compound Data

Melting point	**81.00 °C**	**354.15 K**			
CSID	21106124	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	185.2218	**H bond donors**	2	**ACD/LogP**	2.53
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.20 g/cm^3
SMILES	Oc2cccc(Nc1ccccc1)c2				
STD InChIKey	NDACNGSDAFKTGE-UHFFFAOYAF				

Melting Points

mp °C	source
80.00	Alfa Aesar
81.50	Oxford University MSDS
81.50	PHYSPROP

3-anisidine C7H9NO[2, 3, 64]



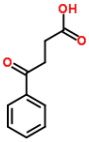
Compound Data

Melting point	**-0.67 °C**	**272.48 K**			
CSID	13869480	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	123.1525	**H bond donors**	2	**ACD/LogP**	0.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	Nc1cccc(OC)c1				
STD InChIKey	NCBZRJODKRCREW-UHFFFAOYAV				

Melting Points

mp °C	source
0.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-1.00	Alfa Aesar
-1.00	PHYSPROP

3-benzoylpropionic acid C10H10O3[3, 64]



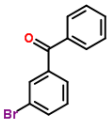
Compound Data

Melting point	**117.50 °C**	**390.65 K**			
CSID	65703	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	178.1846	**H bond donors**	1	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	O=C(c1ccccc1)CCC(=O)O				
STD InChIKey	KMQLIDDEQAJAGJ-UHFFFAOYAS				

Melting Points

mp °C	source
117.00	Alfa Aesar
118.00	PHYSPROP

3-brombenzophenone C13H9BrO[3, 64]



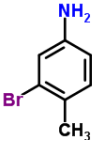
Compound Data

Melting point	**78.50 °C**	**351.65 K**			
CSID	63718	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	261.114	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.42 g/cm^3
SMILES	O=C(c1cc(Br)ccc1)c2ccccc2				
STD InChIKey	XNUMUNIJQMSNNN-UHFFFAOYAU				

Melting Points

mp °C	source
76.00	Alfa Aesar
81.00	PHYSPROP

3-bromo-4-methylaniline C7H8BrN[3, 64]



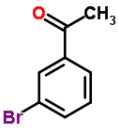
Compound Data

Melting point	**26.50 °C**	**299.65 K**			
CSID	74169	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	186.0491	**H bond donors**	2	**ACD/LogP**	2.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.50 g/cm^3
SMILES	Brc1cc(N)ccc1C				
STD InChIKey	GRXMMIBZRMKADT-UHFFFAOYAE				

Melting Points

mp °C	source
27.00	Alfa Aesar
26.00	PHYSPROP

3-bromoacetophenone C8H7BrO[3, 64]



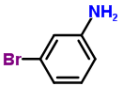
Compound Data

Melting point	**7.75 °C**	**280.90 K**			
CSID	15644	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	199.0446	**H bond donors**	0	**ACD/LogP**	2.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.45 g/cm^3
SMILES	O=C(c1cc(Br)ccc1)C				
STD InChIKey	JYAQYXOVOHJRCS-UHFFFAOYAF				

Melting Points

mp °C	source
8.00	Alfa Aesar
7.50	PHYSPROP

3-bromoaniline C6H6BrN[2, 3, 64]



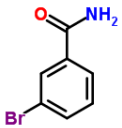
Compound Data

Melting point	**17.17 °C**	**290.32 K**			
CSID	13860633	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	172.0225	**H bond donors**	2	**ACD/LogP**	2.10
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.59 g/cm^3
SMILES	Nc1cc(Br)ccc1				
STD InChIKey	DHYHYLGCQVVLOQ-UHFFFAOYAY				

Melting Points

mp °C	source
17.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
16.00	Alfa Aesar
18.50	PHYSPROP

3-bromobenzamide C7H6BrNO[7, 64]



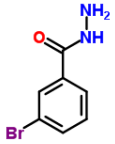
Compound Data

Melting point	**155.15 °C**	**428.30 K**			
CSID	81061	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.0326	**H bond donors**	2	**ACD/LogP**	1.65
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.61 g/cm^3
SMILES	O=C(c1cc(Br)ccc1)N				
STD InChIKey	ODJFDWIECLJWSR-UHFFFAOYAG				

Melting Points

mp °C	source
155.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
155.30	PHYSPROP

3-bromobenzhydrazide C7H7BrN2O[3, 64]



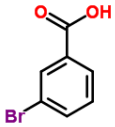
Compound Data

Melting point	**157.00 °C**	**430.15 K**			
CSID	454393	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	215.0473	**H bond donors**	3	**ACD/LogP**	1.26
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.61 g/cm^3
SMILES	O=C(c1cc(Br)ccc1)NN				
STD InChIKey	BNAQRAZIPAHWAR-UHFFFAOYAG				

Melting Points

mp °C	source
156.00	Alfa Aesar
158.00	PHYSPROP

3-bromobenzoic acid C7H5BrO2[2, 3, 64, 70]



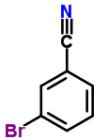
Compound Data

Melting point	**156.00 °C**	**429.15 K**			
CSID	10972	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	201.0174	**H bond donors**	1	**ACD/LogP**	2.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.70 g/cm^3
SMILES	O=C(O)c1cc(Br)ccc1				
STD InChIKey	VOIZNVUXCQLQHS-UHFFFAOYAC				

Melting Points

mp °C	source
157.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
155.00	Alfa Aesar
155.00	PHYSPROP
157.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

3-bromobenzonitrile C7H4BrN[2, 3, 64]



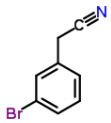
Compound Data

Melting point	**39.17 °C**	**312.32 K**			
CSID	21865	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.0174	**H bond donors**	0	**ACD/LogP**	2.14
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.60 g/cm^3
SMILES	N#Cc1cc(Br)ccc1				
STD InChIKey	STXAVEHFKAXGOX-UHFFFAOYAU				

Melting Points

mp °C	source
39.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
39.00	Alfa Aesar
39.50	PHYSPROP

3-bromobenzyl cyanide C_8H_6BrN[2, 3]



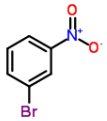
Compound Data

Melting point	**27.50 °C**	**300.65 K**			
CSID	33137	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.0439	**H bond donors**	0	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.49 g/cm^3
SMILES	Brc1cc(ccc1)CC#N				
STD InChIKey	UUZYFBXKWIQKTF-UHFFFAOYAN				

Melting Points

mp °C	source
28.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
27.00	Alfa Aesar

3-bromonitrobenzene $C_6H_4BrNO_2$[2, 64]



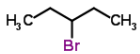
Compound Data

Melting point	**55.00 °C**	**328.15 K**			
CSID	21111786	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	202.0055	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.72 g/cm^3
SMILES	O=[N+]([O-])c1cc(Br)ccc1				
STD InChIKey	FWIROFMBWVMWLB-UHFFFAOYAI				

Melting Points

mp °C	source
54.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
56.00	PHYSPROP

3-bromopentane $C_5H_{11}Br$[31, 64]



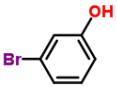
Compound Data

Melting point	**-126.10 °C**	**147.05 K**			
CSID	14966	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	151.0448	**H bond donors**	0	**ACD/LogP**	3.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	BrC(CC)CC				
STD InChIKey	VTOQFOCYBTVOJZ-UHFFFAOYAL				

Melting Points

mp °C	source
-126.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-126.20	PHYSPROP

3-bromophenol C_6H_5BrO[2, 3, 64]



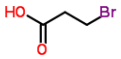
Compound Data

Melting point	**31.33 °C**	**304.48 K**			
CSID	13875441	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	173.0073	**H bond donors**	1	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.66 g/cm^3
SMILES	Oc1cc(Br)ccc1				
STD InChIKey	MNOJRWOWILAHAV-UHFFFAOYAF				

Melting Points

mp °C	source
31.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
30.00	Alfa Aesar
33.00	PHYSPROP

3-bromopropionic acid C3H5BrO2[3, 64]



Compound Data

Melting point	**61.25 °C**	**334.40 K**			
CSID	11066	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	152.9746	**H bond donors**	1	**ACD/LogP**	0.69
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.78 g/cm^3
SMILES	BrCCC(=O)O				
STD InChIKey	DHXNZYCXMFBMHE-UHFFFAOYAK				

Melting Points

mp °C	source
60.00	Alfa Aesar
62.50	PHYSPROP

3-bromopyridine C5H4BrN[3, 64]

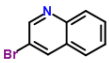
Compound Data

Melting point	**-27.15 °C**	**246.00 K**			
CSID	11783	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	157.996	**H bond donors**	0	**ACD/LogP**	1.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.60 g/cm^3
SMILES	Brc1cccnc1				
STD InChIKey	NYPYPOZNGOXYSU-UHFFFAOYAJ				

Melting Points

mp °C	source
-27.00	Alfa Aesar
-27.30	PHYSPROP

3-bromoquinoline C9H6BrN[3, 64]



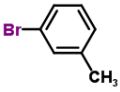
Compound Data

Melting point	**13.65 °C**	**286.80 K**			
CSID	20124	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	208.0546	**H bond donors**	0	**ACD/LogP**	3.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.56 g/cm^3
SMILES	Brc1cc2ccccc2nc1				
STD InChIKey	ZGIKWINFUGEQEO-UHFFFAOYAK				

Melting Points

mp °C	source
14.00	Alfa Aesar
13.30	PHYSPROP

3-bromotoluene C7H7Br[2, 3, 64]



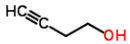
Compound Data

Melting point	**-39.93 °C**	**233.22 K**			
CSID	13875392	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	171.0345	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	Cc1cc(Br)ccc1				
STD InChIKey	WJIFKOVZNJTSGO-UHFFFAOYAY				

Melting Points

mp °C	source
-40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-40.00	Alfa Aesar
-39.80	PHYSPROP

3-butyn-1-ol C4H6O[3, 61, 64]



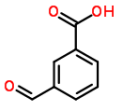
Compound Data

Melting point	**-63.40 °C**	**209.75 K**			
CSID	12977	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	70.0898	**H bond donors**	1	**ACD/LogP**	0.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.92 g/cm^3
SMILES	C#CCCO				
STD InChIKey	OTJZCIYGRUNXTP-UHFFFAOYAH				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-63.60	Oxford University MSDS
-63.60	PHYSPROP

3-carboxybenzaldehyde C8H6O3[3, 7, 64, 64]



Compound Data

Melting point	**174.33 °C**	**447.48 K**			
CSID	11580	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1314	**H bond donors**	1	**ACD/LogP**	1.60
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)c1cccc(C=O)c1				
STD InChIKey	UHDNUPHSDMOGCR-UHFFFAOYAK				

Melting Points

mp °C	source
174.00	Alfa Aesar
175.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
174.00	PHYSPROP
	Values not used in calculating the average melting point
247.00	PHYSPROP[1]

1. wrong isomer JCB

3-chloro-2-methylaniline C7H8ClN[3, 64]

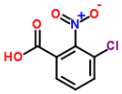
Compound Data

Melting point	**1.50 °C**	**274.65 K**			
CSID	6628	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	141.5981	**H bond donors**	2	**ACD/LogP**	2.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Clc1cccc(N)c1C				
STD InChIKey	ZUVPLKVDZNDZCM-UHFFFAOYAZ				

Melting Points

mp °C	source
2.00	Alfa Aesar
1.00	PHYSPROP

3-chloro-2-nitrobenzoic acid C7H4ClNO4[2, 3, 64]



Compound Data

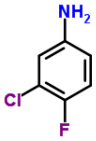
Melting point	**237.33 °C**	**510.48 K**			
CSID	19663	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	1	**ACD/LogP**	2.36
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=[N+]([O-])c1c(cccc1Cl)C(=O)O				
STD InChIKey	VCHSXYHBMFKRBK-UHFFFAOYAV				

Melting Points

mp °C	source
237.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
237.00	Alfa Aesar

238.00	PHYSPROP

3-chloro-4-fluoroaniline C6H5ClFN[3, 61, 64]



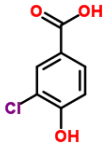
Compound Data

Melting point	**45.67 °C**	**318.82 K**			
CSID	9327	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	145.562	**H bond donors**	2	**ACD/LogP**	2.14
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	Fc1ccc(N)cc1Cl				
STD InChIKey	YSEMCVGMNUUNRK-UHFFFAOYAD				

Melting Points

mp °C	source
46.00	Alfa Aesar
45.50	Oxford University MSDS
45.50	PHYSPROP

3-chloro-4-hydroxybenzoic acid C7H5ClO3[3, 64]



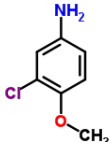
Compound Data

Melting point	**170.00 °C**	**443.15 K**			
CSID	18708	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	172.5658	**H bond donors**	2	**ACD/LogP**	2.39
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.54 g/cm^3
SMILES	Clc1cc(C(=O)O)ccc1O				
STD InChIKey	QGNLHMKIGMZKJX-UHFFFAOYAR				

Melting Points

mp °C	source
169.00	Alfa Aesar
171.00	PHYSPROP

3-chloro-4-methoxyaniline C7H8ClNO[2, 64]



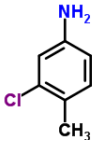
Compound Data

Melting point	**51.25 °C**	**324.40 K**			
CSID	20151	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	157.5975	**H bond donors**	2	**ACD/LogP**	1.57
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	Clc1cc(ccc1OC)N				
STD InChIKey	XQVCBOLNTSUFGD-UHFFFAOYAN				

Melting Points

mp °C	source
50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
52.50	PHYSPROP

3-chloro-4-methylaniline C7H8ClN[3, 61, 64]



Compound Data

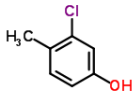
Melting point	**25.00 °C**	**298.15 K**			
CSID	6985	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	141.5981	**H bond donors**	2	**ACD/LogP**	2.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Clc1cc(N)ccc1C				
STD InChIKey	RQKFYFNZSHWXAW-UHFFFAOYAO				

Melting Points

mp °C	source
23.00	Alfa Aesar
26.00	Oxford University MSDS

26.00	PHYSPROP

3-chloro-4-methylphenol C7H7ClO[3, 64]



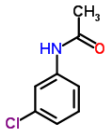
Compound Data

Melting point	**53.75 °C**	**326.90 K**			
CSID	14163	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	142.5829	**H bond donors**	1	**ACD/LogP**	2.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	Clc1cc(O)ccc1C				
STD InChIKey	VQZRLBWPEHFGCD-UHFFFAOYAO				

Melting Points

mp °C	source
52.00	Alfa Aesar
55.50	PHYSPROP

3-chloroacetanilide C8H8ClNO[3, 64]



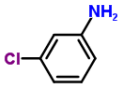
Compound Data

Melting point	**78.50 °C**	**351.65 K**			
CSID	11009	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	169.6082	**H bond donors**	1	**ACD/LogP**	1.81
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	Clc1cc(NC(=O)C)ccc1				
STD InChIKey	MUUQHCOAOLLHIL-UHFFFAOYAA				

Melting Points

mp °C	source
77.00	Alfa Aesar
80.00	PHYSPROP

3-chloroaniline C6H6ClN[3, 31, 64]



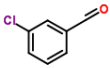
Compound Data

Melting point	**-10.13 °C**	**263.02 K**			
CSID	13869451	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	127.5715	**H bond donors**	2	**ACD/LogP**	1.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	Nc1cc(Cl)ccc1				
STD InChIKey	PNPCRKVUWYDDST-UHFFFAOYAH				

Melting Points

mp °C	source
-10.00	Alfa Aesar
-10.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-10.40	PHYSPROP

3-chlorobenzaldehyde C7H5ClO[2, 3, 64]



Compound Data

Melting point	**17.50 °C**	**290.65 K**			
CSID	21111819	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	140.567	**H bond donors**	0	**ACD/LogP**	2.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	O=Cc1cc(Cl)ccc1				
STD InChIKey	SRWILAKSARHZPR-UHFFFAOYAM				

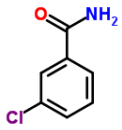
Melting Points

mp °C	source
18.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
17.00	Alfa Aesar

17.50	PHYSPROP

3-chlorobenzamide C7H6ClNO[3, 7]

Compound Data



Melting point	**135.50 °C**	**408.65 K**			
CSID	62467	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	155.5816	**H bond donors**	2	**ACD/LogP**	1.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1cc(Cl)ccc1)N				
STD InChIKey	MJTGQALMWUUPQM-UHFFFAOYAL				

Melting Points

mp °C	source
135.00	Alfa Aesar
136.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

3-chlorobenzamide C8H9NO[2, 3, 64]

Compound Data

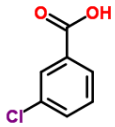
Melting point	**95.33 °C**	**368.48 K**			
CSID	62466	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	2	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	O=C(c1cc(ccc1)C)N				
STD InChIKey	WGRPQCFFBRDZFV-UHFFFAOYAT				

Melting Points

mp °C	source
96.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
95.00	Alfa Aesar
95.00	PHYSPROP

3-chlorobenzoic acid C7H5ClO2[2, 3, 64]

Compound Data



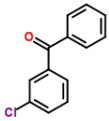
Melting point	**157.00 °C**	**430.15 K**			
CSID	434	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.5664	**H bond donors**	1	**ACD/LogP**	2.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	O=C(O)c1cc(Cl)ccc1				
STD InChIKey	LULAYUGMBFYYEX-UHFFFAOYAK				

Melting Points

mp °C	source
156.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
157.00	Alfa Aesar
158.00	PHYSPROP

3-chlorobenzophenone C13H9ClO[2, 3]

Compound Data



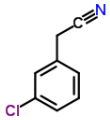
Melting point	**82.50 °C**	**355.65 K**			
CSID	59487	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	216.663	**H bond donors**	0	**ACD/LogP**	3.98
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	O=C(c1cc(Cl)ccc1)c2ccccc2				
STD InChIKey	CPLWKNRPZVNELG-UHFFFAOYAS				

Melting Points

mp °C	source
82.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

83.00	Alfa Aesar

3-chlorobenzyl cyanide C8H6ClN[3, 61]



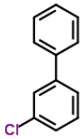
Compound Data

Melting point	**11.75 °C**	**284.90 K**			
CSID	66365	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	151.5929	**H bond donors**	0	**ACD/LogP**	2.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.19 g/cm^3
SMILES	Clc1cc(ccc1)CC#N				
STD InChIKey	GTIKLPYCSAMPNG-UHFFFAOYAY				

Melting Points

mp °C	source
12.00	Alfa Aesar
11.50	Oxford University MSDS

3-chlorobiphenyl C12H9Cl[7, 64]



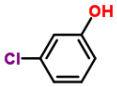
Compound Data

Melting point	**17.00 °C**	**290.15 K**			
CSID	15488	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	188.6529	**H bond donors**	0	**ACD/LogP**	4.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	Clc2cc(c1ccccc1)ccc2				
STD InChIKey	NMWSKOLWZZWHPL-UHFFFAOYAE				

Melting Points

mp °C	source
18.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
16.00	PHYSPROP

3-chlorophenol C6H5ClO[2, 3, 32, 61, 64, 72]



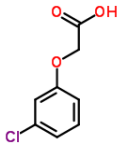
Compound Data

Melting point	**32.93 °C**	**306.08 K**			
CSID	13875432	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	128.5563	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Oc1cc(Cl)ccc1				
STD InChIKey	HORNXRXVQWOLPJ-UHFFFAOYAL				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar
32.60	DrugBank
33.00	Oxford University MSDS
33.50	PHYSPROP
32.50	Sigma-Aldrich

3-chlorophenoxyacetic acid C8H7ClO3[3, 64]



Compound Data

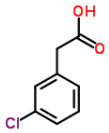
Melting point	**109.00 °C**	**382.15 K**			
CSID	11013	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	186.5924	**H bond donors**	1	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.37 g/cm^3
SMILES	Clc1cc(OCC(=O)O)ccc1				
STD InChIKey	XSBUXVWJQVTYLC-UHFFFAOYAT				

Melting Points

mp °C	source
108.00	Alfa Aesar
110.00	PHYSPROP

3-chlorophenylacetic acid C8H7ClO2[2, 3, 64]

Compound Data



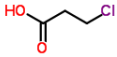
Melting point	**78.58 °C**	**351.73 K**			
CSID	15092	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	170.593	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	Clc1cc(ccc1)CC(=O)O				
STD InChIKey	WFPMUFXQDKMVCO-UHFFFAOYAR				

Melting Points

mp °C	source
78.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
79.00	Alfa Aesar
78.75	PHYSPROP

3-chloropropionic acid C3H5ClO2[3, 64]

Compound Data



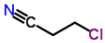
Melting point	**40.00 °C**	**313.15 K**			
CSID	7611	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.5236	**H bond donors**	1	**ACD/LogP**	0.41
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.29 g/cm^3
SMILES	ClCCC(=O)O				
STD InChIKey	QEYMMOKECZBKAC-UHFFFAOYAJ				

Melting Points

mp °C	source
39.00	Alfa Aesar
41.00	PHYSPROP

3-chloropropionitrile C3H4ClN[2, 3, 64]

Compound Data



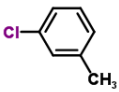
Melting point	**-50.67 °C**	**222.48 K**			
CSID	10498	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	89.5236	**H bond donors**	0	**ACD/LogP**	0.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	ClCCC#N				
STD InChIKey	GNHMRTZZNHZDDM-UHFFFAOYAG				

Melting Points

mp °C	source
-50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-51.00	Alfa Aesar
-51.00	PHYSPROP

3-chlorotoluene C7H7Cl[2, 3, 61, 64]

Compound Data



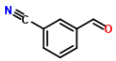
Melting point	**-47.95 °C**	**225.20 K**			
CSID	13875230	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	126.5835	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	Cc1cc(Cl)ccc1				
STD InChIKey	OSOUNOBYRMOXQQ-UHFFFAOYAB				

Melting Points

mp °C	source
-48.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-48.00	Alfa Aesar
-48.00	Oxford University MSDS
-47.80	PHYSPROP

3-cyanobenzaldehyde C8H5NO[2, 3, 64]

Compound Data



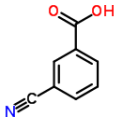
Melting point	**76.83 °C**	**349.98 K**			
CSID	21112367	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	131.1314	**H bond donors**	0	**ACD/LogP**	1.18
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	N#Cc1cccc(C=O)c1				
STD InChIKey	HGZJJKZPPMFIBU-UHFFFAOYAM				

Melting Points

mp °C	source
77.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
77.00	Alfa Aesar
76.50	PHYSPROP

3-cyanobenzoic acid C8H5NO2[2, 3, 64]

Compound Data



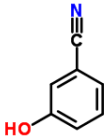
Melting point	**221.33 °C**	**494.48 K**			
CSID	15088	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	147.1308	**H bond donors**	1	**ACD/LogP**	1.48
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	N#Cc1cc(C(=O)O)ccc1				
STD InChIKey	GYLKKXHEIIFTJH-UHFFFAOYAK				

Melting Points

mp °C	source
223.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
222.00	Alfa Aesar
219.00	PHYSPROP

3-cyanophenol C7H5NO[2, 3, 64, 72]

Compound Data



Melting point	**80.38 °C**	**353.52 K**			
CSID	12821	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	119.1207	**H bond donors**	1	**ACD/LogP**	1.70
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	N#Cc1cc(O)ccc1				
STD InChIKey	SGHBRHKBCLLVCI-UHFFFAOYAD				

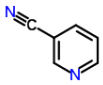
Melting Points

mp °C	source
82.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
80.00	Alfa Aesar
80.00	PHYSPROP
79.50	Sigma-Aldrich

3-cyanopyridine C6H4N2[3, 61, 64]

Compound Data

Melting point	**50.33 °C**	**323.48 K**			
CSID	78	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	104.1094	**H bond donors**	0	**ACD/LogP**	0.42
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	3



1.12 g/cm

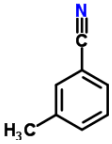
SMILES	c1cc(cnc1)C#N
STD InChIKey	GZPHSAQLYPIAIN-UHFFFAOYAR

Melting Points

mp °C	source
50.00	Alfa Aesar
50.00	Oxford University MSDS
51.00	PHYSPROP

3-cyanotoluene C8H7N[2, 3, 64]

Compound Data



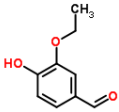
Melting point	**-24.33 °C**	**248.82 K**			
CSID	11607	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	117.1479	**H bond donors**	0	**ACD/LogP**	2.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	N#Cc1cccc(c1)C				
STD InChIKey	BOHCMQZJWOGWTA-UHFFFAOYAY				

Melting Points

mp °C	source
-23.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-27.00	Alfa Aesar
-23.00	PHYSPROP

3-ethoxy-4-hydroxybenzaldehyde C9H10O3[3, 64]

Compound Data



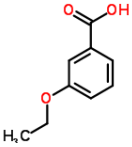
Melting point	**77.25 °C**	**350.40 K**			
CSID	8154	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	1.72
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.19 g/cm^3
SMILES	O=Cc1cc(OCC)c(O)cc1				
STD InChIKey	CBOQJANXLMLOSS-UHFFFAOYAD				

Melting Points

mp °C	source
77.00	Alfa Aesar
77.50	PHYSPROP

3-ethoxybenzoic acid C9H10O3[3, 64]

Compound Data



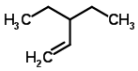
Melting point	**136.50 °C**	**409.65 K**			
CSID	11628	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	2.55
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)c1cc(OCC)ccc1				
STD InChIKey	DTFQMPQJMDEWKJ-UHFFFAOYAC				

Melting Points

mp °C	source
136.00	Alfa Aesar
137.00	PHYSPROP

3-ethyl-1-pentene C7H14[4, 64]

Compound Data



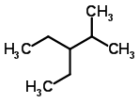
Melting point	**-127.25 °C**	**145.90 K**			
CSID	18792	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.78
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.70 g/cm^3
SMILES	C=C\C(CC)CC				
STD InChIKey	YPVPQMCSLFDIKA-UHFFFAOYAR				

Melting Points

mp °C	source
-127.00	American Petroleum Institute. Research Project 44; Selected ...
-127.50	PHYSPROP

3-ethyl-2-methylpentane C8H18[4, 64]

Compound Data



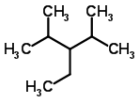
Melting point	**-114.95 °C**	**158.20 K**			
CSID	11370	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.64
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)C(CC)CC				
STD InChIKey	DUPUVYJQZSLSJB-UHFFFAOYAR				

Melting Points

mp °C	source
-115.00	American Petroleum Institute. Research Project 44; Selected ...
-114.90	PHYSPROP

3-ethyl-2,4-dimethylpentane C9H20[4, 64]

Compound Data



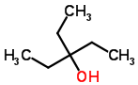
Melting point	**-122.20 °C**	**150.95 K**			
CSID	13421	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	4.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.72 g/cm^3
SMILES	CC(C)C(CC)C(C)C				
STD InChIKey	VLHAGZNBWKUMRW-UHFFFAOYAK				

Melting Points

mp °C	source
-122.00	American Petroleum Institute. Research Project 44; Selected ...
-122.40	PHYSPROP

3-ethyl-3-pentanol C7H16O[3, 64]

Compound Data



Melting point	**-12.75 °C**	**260.40 K**			
CSID	11210	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	116.2013	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.82 g/cm^3
SMILES	OC(CC)(CC)CC				
STD InChIKey	XKIRHOWVQWCYBT-UHFFFAOYAB				

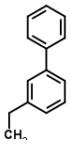
Melting Points

mp °C	source
-13.00	Alfa Aesar
-12.50	PHYSPROP

3-ethylbiphenyl C14H14[4, 64]

Compound Data

Melting point	**-27.75 °C**	**245.40 K**			
CSID	72051	**H bond acceptors**	0	**Rule of 5 violations**	0

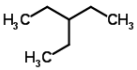


Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.97
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	c2(c1cccc(c1)CC)ccccc2				
STD InChIKey	HUXKTWJQSHBZIV-UHFFFAOYAH				

Melting Points

mp °C	source
-28.00	American Petroleum Institute. Research Project 44; Selected ...
-27.50	PHYSPROP

3-ethylpentane C7H16[4, 64]



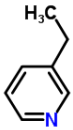
Compound Data

Melting point	**-118.80 °C**	**154.35 K**			
CSID	11551	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.2019	**H bond donors**	0	**ACD/LogP**	4.29
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.69 g/cm^3
SMILES	CCC(CC)CC				
STD InChIKey	AORMDLNPRGXHHL-UHFFFAOYAP				

Melting Points

mp °C	source
-119.00	American Petroleum Institute. Research Project 44; Selected ...
-118.60	PHYSPROP

3-ethylpyridine C7H9N[3, 64]



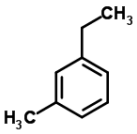
Compound Data

Melting point	**-76.95 °C**	**196.20 K**			
CSID	21105905	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	0	**ACD/LogP**	1.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.93 g/cm^3
SMILES	CCc1cccnc1				
STD InChIKey	MFEIKQPHQINPRI-UHFFFAOYAR				

Melting Points

mp °C	source
-77.00	Alfa Aesar
-76.90	PHYSPROP

3-ethyltoluene C9H12[3, 4, 64]



Compound Data

Melting point	**-95.83 °C**	**177.32 K**			
CSID	11603	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.1916	**H bond donors**	0	**ACD/LogP**	3.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1ccc(cc1CC)C				
STD InChIKey	ZLCSFXXPPANWQY-UHFFFAOYAP				

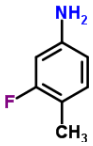
Melting Points

mp °C	source
-96.00	Alfa Aesar
-96.00	American Petroleum Institute. Research Project 44; Selected ...
-95.50	PHYSPROP

3-fluoro-4-methylaniline C7H8FN[3, 64]

Compound Data

Melting point	**32.00 °C**	**305.15 K**



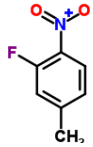
CSID	9563	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	125.1435	**H bond donors**	2	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	Fc1c(ccc(N)c1)C				
STD InChIKey	MGRHBBRSAFPBIN-UHFFFAOYAI				

Melting Points

mp °C	source
33.00	Alfa Aesar
31.00	PHYSPROP

3-fluoro-4-nitrotoluene C7H6FNO2[3, 64]

Compound Data



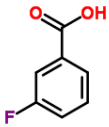
Melting point	**53.10 °C**	**326.25 K**			
CSID	61281	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	155.1264	**H bond donors**	0	**ACD/LogP**	2.15
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	O=[N+]([O-])c1ccc(cc1F)C				
STD InChIKey	WZMOWQCNPFDWPA-UHFFFAOYAV				

Melting Points

mp °C	source
53.00	Alfa Aesar
53.20	PHYSPROP

3-fluorobenzoic acid C7H5FO2[3, 64]

Compound Data



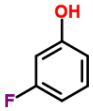
Melting point	**123.50 °C**	**396.65 K**			
CSID	9574	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	140.1118	**H bond donors**	1	**ACD/LogP**	2.16
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)c1cc(F)ccc1				
STD InChIKey	MXNBDFWNYRNIBH-UHFFFAOYAD				

Melting Points

mp °C	source
123.00	Alfa Aesar
124.00	PHYSPROP

3-fluorophenol C6H5FO[3, 61, 64]

Compound Data



Melting point	**11.90 °C**	**285.05 K**			
CSID	9360	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	112.1017	**H bond donors**	1	**ACD/LogP**	1.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	Fc1cccc(O)c1				
STD InChIKey	SJTBRFHBXDZMPS-UHFFFAOYAM				

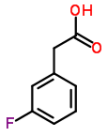
Melting Points

mp °C	source
12.00	Alfa Aesar
10.00	Oxford University MSDS
13.70	PHYSPROP

3-fluorophenylacetic acid C8H7FO2[3, 64]

Compound Data

Melting point	**44.50 °C**	**317.65 K**



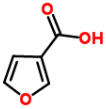
CSID	60937	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	154.1384	**H bond donors**	1	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	Fc1cc(ccc1)CC(=O)O				
STD InChIKey	YEAUYVGUXSZCFI-UHFFFAOYAP				

Melting Points

mp °C	source
46.00	Alfa Aesar
43.00	PHYSPROP

3-furoic acid C5H4O3[3, 64]

Compound Data



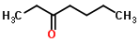
Melting point	**122.25 °C**	**395.40 K**			
CSID	9849	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	112.0835	**H bond donors**	1	**ACD/LogP**	1.03
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	c1cocc1C(=O)O				
STD InChIKey	IHCCAYCGZOLTEU-UHFFFAOYAX				

Melting Points

mp °C	source
122.00	Alfa Aesar
122.50	PHYSPROP

3-heptanone C7H14O[3, 4, 61, 64]

Compound Data



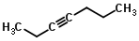
Melting point	**-38.50 °C**	**234.65 K**			
CSID	7514	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	114.1855	**H bond donors**	0	**ACD/LogP**	1.97
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.81 g/cm^3
SMILES	O=C(CC)CCCC				
STD InChIKey	NGAZZOYFWWSOGK-UHFFFAOYAV				

Melting Points

mp °C	source
-37.00	Alfa Aesar
-39.00	American Petroleum Institute. Research Project 44; Selected ...
-39.00	Oxford University MSDS
-39.00	PHYSPROP

3-heptyne C7H12[4, 64]

Compound Data



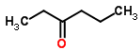
Melting point	**-130.75 °C**	**142.40 K**			
CSID	68268	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	3.05
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.75 g/cm^3
SMILES	C(#CCCC)CC				
STD InChIKey	KLYHSJRCIZOUHE-UHFFFAOYAH				

Melting Points

mp °C	source
-131.00	American Petroleum Institute. Research Project 44; Selected ...
-130.50	PHYSPROP

3-hexanone C6H12O[3, 64]

Compound Data



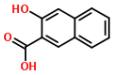
Melting point	**-55.25 °C**	**217.90 K**			
CSID	11025	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	100.1589	**H bond donors**	0	**ACD/LogP**	1.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.80 g/cm^3
SMILES	O=C(CC)CCC				
STD InChIKey	PFCHFHIRKBAQGU-UHFFFAOYAM				

Melting Points

mp °C	source
-55.00	Alfa Aesar
-55.50	PHYSPROP

3-hydroxy-2-naphthoic acid C11H8O3[3, 64]

Compound Data



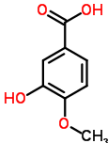
Melting point	**221.25 °C**	**494.40 K**			
CSID	6837	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	188.1794	**H bond donors**	2	**ACD/LogP**	3.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.40 g/cm^3
SMILES	O=C(O)c2cc1c(cccc1)cc2O				
STD InChIKey	ALKYHXVLJMQRLQ-UHFFFAOYAT				

Melting Points

mp °C	source
220.00	Alfa Aesar
222.50	PHYSPROP

3-hydroxy-4-methoxybenzoic acid C8H8O4[3, 64]

Compound Data



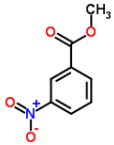
Melting point	**252.25 °C**	**525.40 K**			
CSID	12055	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	2	**ACD/LogP**	1.35
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.35 g/cm^3
SMILES	O=C(O)c1ccc(OC)c(O)c1				
STD InChIKey	LBKFGYZQBSGRHY-UHFFFAOYAM				

Melting Points

mp °C	source
253.00	Alfa Aesar
251.50	PHYSPROP

3-hydroxy-4-nitrobenzoic acid C8H7NO4[2, 3, 61, 64]

Compound Data



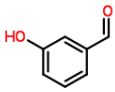
Melting point	**78.75 °C**	**351.90 K**			
CSID	62472	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	181.1455	**H bond donors**	0	**ACD/LogP**	1.82
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.30 g/cm^3
SMILES	O=[N+]([O-])c1cc(C(=O)OC)ccc1				
STD InChIKey	AXLYJLKKPUICKV-UHFFFAOYAV				

Melting Points

mp °C	source
80.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
79.00	Alfa Aesar
78.00	Oxford University MSDS
78.00	PHYSPROP

3-hydroxybenzaldehyde C7H6O2[2, 3, 64]

Compound Data



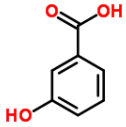
Melting point	**105.67 °C**	**378.82 K**			
CSID	21105795	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1213	**H bond donors**	1	**ACD/LogP**	1.25
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=Cc1cc(O)ccc1				
STD InChIKey	IAVREABSGIHHMO-UHFFFAOYAC				

Melting Points

mp °C	source
105.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
104.00	Alfa Aesar
108.00	PHYSPROP

3-hydroxybenzoic acid C7H6O3[2, 3, 64]

Compound Data



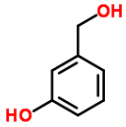
Melting point	**202.33 °C**	**475.48 K**			
CSID	7142	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	138.1207	**H bond donors**	2	**ACD/LogP**	1.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.38 g/cm^3
SMILES	O=C(O)c1cc(O)ccc1				
STD InChIKey	IJFXRHURBJZNAO-UHFFFAOYAV				

Melting Points

mp °C	source
203.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
202.00	Alfa Aesar
202.00	PHYSPROP

3-hydroxybenzyl alcohol C7H8O2[2, 3, 64]

Compound Data



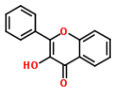
Melting point	**72.00 °C**	**345.15 K**			
CSID	100	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	0.50
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	c1cc(cc(c1)O)CO				
STD InChIKey	OKVJCVWFVRATSG-UHFFFAOYAA				

Melting Points

mp °C	source
72.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
71.00	Alfa Aesar
73.00	PHYSPROP

3-hydroxyflavone C15H10O3[3, 64]

Compound Data

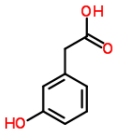


Melting point	**170.75 °C**	**443.90 K**			
CSID	10871	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	238.2381	**H bond donors**	1	**ACD/LogP**	3.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.37 g/cm^3
SMILES	O=C1c3c(O/C(=C1/O)c2ccccc2)cccc3				
STD InChIKey	HVQAJTFOCKOKIN-UHFFFAOYAX				

Melting Points

mp °C	source
170.00	Alfa Aesar
171.50	PHYSPROP

3-hydroxyphenylacetic acid C8H8O3[3, 64]



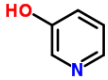
Compound Data

Melting point	**131.00 °C**	**404.15 K**			
CSID	11624	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)Cc1cc(O)ccc1				
STD InChIKey	FVMDYYGIDFPZAX-UHFFFAOYAR				

Melting Points

mp °C	source
130.00	Alfa Aesar
132.00	PHYSPROP

3-hydroxypyridine C5H5NO[3, 64]



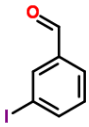
Compound Data

Melting point	**127.25 °C**	**400.40 K**			
CSID	7683	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	95.0993	**H bond donors**	1	**ACD/LogP**	0.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	Oc1cccnc1				
STD InChIKey	GRFNBEZIAWKNCO-UHFFFAOYAT				

Melting Points

mp °C	source
127.00	Alfa Aesar
127.50	PHYSPROP

3-iodobenzaldehyde C7H5IO[3, 7]



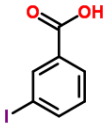
Compound Data

Melting point	**57.00 °C**	**330.15 K**			
CSID	221355	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	232.0185	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.88 g/cm^3
SMILES	O=Cc1cc(I)ccc1				
STD InChIKey	RZODAQZAFOBFLS-UHFFFAOYAZ				

Melting Points

mp °C	source
56.00	Alfa Aesar
58.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

3-iodobenzoic acid C7H5IO2[2, 3, 64]



Compound Data

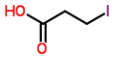
Melting point	**187.43 °C**	**460.58 K**			
CSID	11563	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	248.0179	**H bond donors**	1	**ACD/LogP**	3.11
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.00 g/cm^3
SMILES	O=C(O)c1cc(I)ccc1				
STD InChIKey	KVBWBCRPWVKFQT-UHFFFAOYAV				

Melting Points

mp °C	source
187.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
187.00	Alfa Aesar
188.30	PHYSPROP

3-iodopropionic acid C3H5IO2[3, 64]

Compound Data



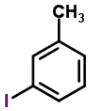
Melting point	**81.75 °C**	**354.90 K**			
CSID	8524	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	199.9751	**H bond donors**	1	**ACD/LogP**	1.04
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.19 g/cm^3
SMILES	ICCC(=O)O				
STD InChIKey	KMRNTNDWADEIIX-UHFFFAOYAY				

Melting Points

mp °C	source
82.00	Alfa Aesar
81.50	PHYSPROP

3-iodotoluene C7H7I[3, 64]

Compound Data



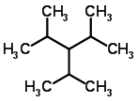
Melting point	**-27.10 °C**	**246.05 K**			
CSID	11765	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	218.0349	**H bond donors**	0	**ACD/LogP**	3.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.71 g/cm^3
SMILES	Ic1cc(ccc1)C				
STD InChIKey	VLCPISYURGTGLP-UHFFFAOYAK				

Melting Points

mp °C	source
-27.00	Alfa Aesar
-27.20	PHYSPROP

3-isopropyl-2,4-dimethylpentane C10H22[4, 64]

Compound Data



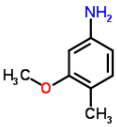
Melting point	**-81.85 °C**	**191.30 K**			
CSID	452568	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.73 g/cm^3
SMILES	CC(C)C(C(C)C)C(C)C				
STD InChIKey	YVYHOOYMDHZALB-UHFFFAOYAK				

Melting Points

mp °C	source
-82.00	American Petroleum Institute. Research Project 44; Selected ...
-81.70	PHYSPROP

3-methoxy-4-methylaniline C8H11NO[3, 64]

Compound Data



Melting point	**57.25 °C**	**330.40 K**			
CSID	25942	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	137.179	**H bond donors**	2	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	O(c1cc(ccc1C)N)C				
STD InChIKey	ONADZNBSLRAJFW-UHFFFAOYAC				

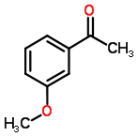
Melting Points

mp °C	source
58.00	Alfa Aesar
56.50	PHYSPROP

3-methoxyacetophenone C9H10O2[3, 19, 64]

Compound Data

Melting point	**-7.50 °C**	**265.65 K**			
CSID	21111758	**H bond acceptors**	2	**Rule of 5 violations**	0



Molecular weight	150.1745	**H bond donors**	0	**ACD/LogP**	1.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	COc1cc(ccc1)C(C)=O				
STD InChIKey	BAYUSCHCCGXLAY-UHFFFAOYAB				

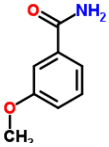
Melting Points

mp °C	source
-7.00	Alfa Aesar
-8.00	Chemical Book
	Values not used in calculating the average melting point
95.50	PHYSPROP[1]

1. clearly out of range JCB

3-methoxybenzamide C8H9NO2[2, 3, 64]

Compound Data



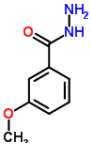
Melting point	**133.33 °C**	**406.48 K**			
CSID	88942	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	0.85
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(c1cc(OC)ccc1)N				
STD InChIKey	VKPLPDIMEREJJF-UHFFFAOYAC				

Melting Points

mp °C	source
133.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
133.00	Alfa Aesar
134.00	PHYSPROP

3-methoxybenzhydrazide C8H10N2O2[3, 64]

Compound Data



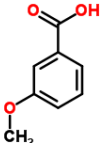
Melting point	**93.00 °C**	**366.15 K**			
CSID	72141	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	166.1772	**H bond donors**	3	**ACD/LogP**	0.38
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3
SMILES	O=C(c1cc(OC)ccc1)NN				
STD InChIKey	VMZSDAQEWPNOIB-UHFFFAOYAX				

Melting Points

mp °C	source
92.00	Alfa Aesar
94.00	PHYSPROP

3-methoxybenzoic acid C8H8O3[2, 3, 64]

Compound Data

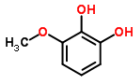


Melting point	**105.33 °C**	**378.48 K**			
CSID	10977	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	2.02
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	O=C(O)c1cc(OC)ccc1				
STD InChIKey	XHQZJYCNDZAGLW-UHFFFAOYAD				

Melting Points

mp °C	source
103.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
106.00	Alfa Aesar
107.00	PHYSPROP

3-methoxycatechol C7H8O3[3, 64]



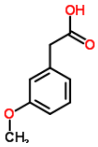
Compound Data

Melting point	**42.40 °C**	**315.55 K**			
CSID	13033	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	140.1366	**H bond donors**	2	**ACD/LogP**	0.70
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	O(c1cccc(O)c1O)C				
STD InChIKey	LPYUENQFPVNPHY-UHFFFAOYAA				

Melting Points

mp °C	source
42.00	Alfa Aesar
42.80	PHYSPROP

3-methoxyphenylacetic acid C9H10O3[3, 64]



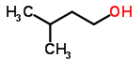
Compound Data

Melting point	**71.00 °C**	**344.15 K**			
CSID	14948	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	1.42
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3
SMILES	O=C(O)Cc1cc(OC)ccc1				
STD InChIKey	LEGPZHPSIPPYIO-UHFFFAOYAY				

Melting Points

mp °C	source
70.00	Alfa Aesar
72.00	PHYSPROP

3-methyl-1-butanol C5H12O[3, 61, 64]



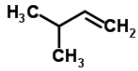
Compound Data

Melting point	**-117.07 °C**	**156.08 K**			
CSID	29000	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	1	**ACD/LogP**	1.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.81 g/cm^3
SMILES	OCCC(C)C				
STD InChIKey	PHTQWCKDNZKARW-UHFFFAOYAW				

Melting Points

mp °C	source
-117.00	Alfa Aesar
-117.00	Oxford University MSDS
-117.20	PHYSPROP

3-methyl-1-butene C5H10[4, 64]



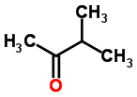
Compound Data

Melting point	**-168.25 °C**	**104.90 K**			
CSID	10765	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.66 g/cm^3
SMILES	C=C\C(C)C				
STD InChIKey	YHQXBTXEYZIYOV-UHFFFAOYAS				

Melting Points

mp °C	source
-168.00	American Petroleum Institute. Research Project 44; Selected ...
-168.50	PHYSPROP

3-methyl-2-butanone C5H10O[3, 4, 64]



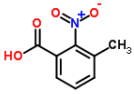
Compound Data

Melting point	**-92.37 °C**	**180.78 K**			
CSID	10777	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	86.1323	**H bond donors**	0	**ACD/LogP**	0.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.79 g/cm^3
SMILES	O=C(C)C(C)C				
STD InChIKey	SYBYTAAJFKOIEJ-UHFFFAOYAE				

Melting Points

mp °C	source
-92.00	Alfa Aesar
-92.00	American Petroleum Institute. Research Project 44; Selected ...
-93.10	PHYSPROP

3-methyl-2-nitrobenzoic acid C8H7NO4[3, 61]



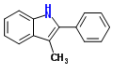
Compound Data

Melting point	**221.50 °C**	**494.65 K**			
CSID	20277	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	181.1455	**H bond donors**	1	**ACD/LogP**	1.81
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	Cc1cccc(c1[N+](=O)[O-])C(=O)O				
STD InChIKey	DGDAVTPQCQXLGU-UHFFFAOYAG				

Melting Points

mp °C	source
222.00	Alfa Aesar
221.00	Oxford University MSDS

3-methyl-2-phenylindole C15H13N[48, 64]



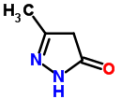
Compound Data

Melting point	**91.25 °C**	**364.40 K**			
CSID	226885	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	207.2704	**H bond donors**	1	**ACD/LogP**	5.14
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	c1cccc3c1c(c(c2ccccc2)n3)C				
STD InChIKey	KYAXCYQVBBQQHB-UHFFFAOYAF				

Melting Points

mp °C	source
91.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
91.50	PHYSPROP

3-methyl-2-pyrazolin-5-one C4H6N2O[3, 64]



Compound Data

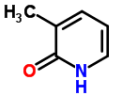
Melting point	**221.50 °C**	**494.65 K**			
CSID	7632	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	98.1032	**H bond donors**	1	**ACD/LogP**	-1.08
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.33 g/cm^3
SMILES	O=C1N/N=C(/C)C1				
STD InChIKey	NHLAPJMCARJFOG-UHFFFAOYAZ				

Melting Points

mp °C	source
222.00	Alfa Aesar
221.00	PHYSPROP

3-methyl-2-pyridone C6H7NO[3, 48, 64]

Compound Data



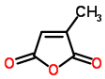
Melting point	**139.83 °C**	**412.98 K**			
CSID	63658	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	1	**ACD/LogP**	0.01
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	O=C1/C(=C\C=C/N1)C				
STD InChIKey	MVKDNXIKAWKCCS-UHFFFAOYAH				

Melting Points

mp °C	source
140.00	Alfa Aesar
138.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
141.50	PHYSPROP

3-methyl-2,5-furandione C5H4O3[3, 64]

Compound Data



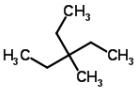
Melting point	**7.75 °C**	**280.90 K**			
CSID	11517	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	112.0835	**H bond donors**	0	**ACD/LogP**	0.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.33 g/cm^3
SMILES	O=C\1OC(=O)/C(=C/1)C				
STD InChIKey	AYKYXWQEBUNJCN-UHFFFAOYAM				

Melting Points

mp °C	source
8.00	Alfa Aesar
7.50	PHYSPROP

3-methyl-3-ethylpentane C8H18[4, 64]

Compound Data



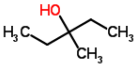
Melting point	**-90.95 °C**	**182.20 K**			
CSID	13400	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.64
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.71 g/cm^3
SMILES	CC(CC)(CC)CC				
STD InChIKey	GIEZWIDCIFCQPS-UHFFFAOYAZ				

Melting Points

mp °C	source
-91.00	American Petroleum Institute. Research Project 44; Selected ...
-90.90	PHYSPROP

3-methyl-3-pentanol C6H14O[4, 64]

Compound Data



Melting point	**-23.80 °C**	**249.35 K**			
CSID	6248	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	102.1748	**H bond donors**	1	**ACD/LogP**	1.57
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.82 g/cm^3
SMILES	OC(C)(CC)CC				
STD InChIKey	FRDAATYAJDYRNW-UHFFFAOYAV				

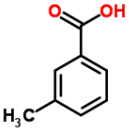
Melting Points

mp °C	source
-24.00	American Petroleum Institute. Research Project 44; Selected ...
-23.60	PHYSPROP

3-methylbenzoic acid C8H8O2[2, 3, 61, 64]

Compound Data

Melting point	**109.92 °C**	**383.07 K**



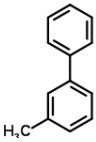
CSID	7140	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	1	**ACD/LogP**	2.35
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	O=C(O)c1cc(ccc1)C				
STD InChIKey	GPSDUZXPYCFOSQ-UHFFFAOYAZ				

Melting Points

mp °C	source
110.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
109.00	Alfa Aesar
112.00	Oxford University MSDS
108.70	PHYSPROP

3-methylbiphenyl C13H12[3, 4, 64]

Compound Data



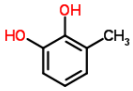
Melting point	**4.83 °C**	**277.98 K**			
CSID	12045	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	168.2344	**H bond donors**	0	**ACD/LogP**	4.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3
SMILES	c2c(c1cccc(c1)C)cccc2				
STD InChIKey	NPDIDUXTRAITDE-UHFFFAOYAC				

Melting Points

mp °C	source
5.00	Alfa Aesar
5.00	American Petroleum Institute. Research Project 44; Selected ...
4.50	PHYSPROP

3-methylcatechol C7H8O2[3, 64]

Compound Data



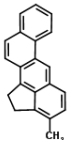
Melting point	**66.50 °C**	**339.65 K**			
CSID	333	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	Oc1c(cccc1O)C				
STD InChIKey	PGSWEKYNAOWQDF-UHFFFAOYAB				

Melting Points

mp °C	source
65.00	Alfa Aesar
68.00	PHYSPROP

3-methylcholanthrene C21H16[44, 61, 64]

Compound Data

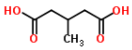


Melting point	**179.67 °C**	**452.82 K**			
CSID	1611	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	268.3517	**H bond donors**	0	**ACD/LogP**	7.11
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.22 g/cm^3
SMILES	c32cc1ccc(c5c1c(c2ccc4ccccc34)CC5)C				
STD InChIKey	PPQNQXQZIWHJRB-UHFFFAOYAO				

Melting Points

mp °C	source
179.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
179.50	Oxford University MSDS
180.00	PHYSPROP

3-methylglutaric acid C6H10O4[3, 64]



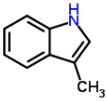
Compound Data

Melting point	**86.50 °C**	**359.65 K**			
CSID	11781	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	146.1412	**H bond donors**	2	**ACD/LogP**	-0.69
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=C(O)CC(C)CC(=O)O				
STD InChIKey	XJMMNTGIMDZPMU-UHFFFAOYAU				

Melting Points

mp °C	source
86.00	Alfa Aesar
87.00	PHYSPROP

3-methylindole C9H9N[3, 61, 64]



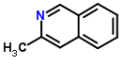
Compound Data

Melting point	**96.17 °C**	**369.32 K**			
CSID	6480	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	131.1745	**H bond donors**	1	**ACD/LogP**	2.60
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c1cccc2c1c(cn2)C				
STD InChIKey	ZFRKQXVRDFCRJG-UHFFFAOYAZ				

Melting Points

mp °C	source
96.00	Alfa Aesar
95.00	Oxford University MSDS
97.50	PHYSPROP

3-methylisoquinoline C10H9N[48, 64]



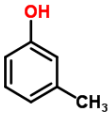
Compound Data

Melting point	**65.50 °C**	**338.65 K**			
CSID	13668	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	0	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	n2c(cc1c(cccc1)c2)C				
STD InChIKey	FVVXWRGARUACNW-UHFFFAOYAG				

Melting Points

mp °C	source
63.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
68.00	PHYSPROP

3-methylphenol C7H8O[3, 31, 32, 61, 64]



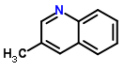
Compound Data

Melting point	**11.52 °C**	**284.67 K**			
CSID	21105871	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	108.1378	**H bond donors**	1	**ACD/LogP**	2.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	Cc1cccc(c1)O				
STD InChIKey	RLSSMJSEOOYNOY-UHFFFAOYAJ				

Melting Points

mp °C	source
11.00	Alfa Aesar
12.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
11.80	DrugBank
11.00	Oxford University MSDS
11.80	PHYSPROP

3-methylquinoline C10H9N[3, 64]



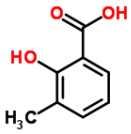
Compound Data

Melting point	**15.75 °C**	**288.90 K**			
CSID	11432	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	n1cc(cc2ccccc12)C				
STD InChIKey	DTBDAFLSBDGPEA-UHFFFAOYAE				

Melting Points

mp °C	source
15.00	Alfa Aesar
16.50	PHYSPROP

3-methylsalicylic acid C8H8O3[3, 64]



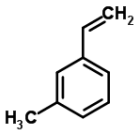
Compound Data

Melting point	**165.25 °C**	**438.40 K**			
CSID	6482	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.30 g/cm^3
SMILES	O=C(O)c1cccc(c1O)C				
STD InChIKey	WHSXTWFYRGOBGO-UHFFFAOYAV				

Melting Points

mp °C	source
165.00	Alfa Aesar
165.50	PHYSPROP

3-methylstyrene C9H10[3, 4, 64]



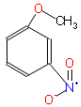
Compound Data

Melting point	**-84.77 °C**	**188.38 K**			
CSID	7248	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.1757	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.90 g/cm^3
SMILES	C=C\c1cc(ccc1)C				
STD InChIKey	JZHGRUMIRATHIU-UHFFFAOYAW				

Melting Points

mp °C	source
-82.00	Alfa Aesar
-86.00	American Petroleum Institute. Research Project 44; Selected ...
-86.30	PHYSPROP

3-nitro-anisole C7H7NO3[2, 64]



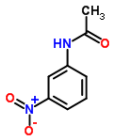
Compound Data

Melting point	**38.25 °C**	**311.40 K**			
CSID	21170967	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	153.1354	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.22 g/cm^3
SMILES	COc1cccc(c1)[N+]([O-])=O				
STD InChIKey	WGYFINWERLNPHR-UHFFFAOYAD				

Melting Points

mp °C	source
38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
38.50	PHYSPROP

3-nitroacetanilide C8H8N2O3[3, 64]



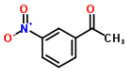
Compound Data

Melting point	**153.50 °C**	**426.65 K**			
CSID	28947	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	180.1607	**H bond donors**	1	**ACD/LogP**	1.47
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=C(Nc1cccc(c1)[N+]([O-])=O)C				
STD InChIKey	KFTYNYHJHKCRKU-UHFFFAOYAG				

Melting Points

mp °C	source
152.00	Alfa Aesar
155.00	PHYSPROP

3-nitroacetophenone C8H7NO3[2, 3, 61, 64]



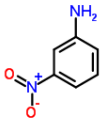
Compound Data

Melting point	**79.50 °C**	**352.65 K**			
CSID	21106145	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	165.1461	**H bond donors**	0	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1)C(C)=O				
STD InChIKey	ARKIFHPFTHVKDT-UHFFFAOYAH				

Melting Points

mp °C	source
78.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
78.00	Alfa Aesar
81.00	Oxford University MSDS
81.00	PHYSPROP

3-nitroaniline C6H6N2O2[2, 3, 64, 72]



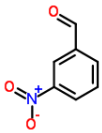
Compound Data

Melting point	**113.38 °C**	**386.52 K**			
CSID	7145	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	138.124	**H bond donors**	2	**ACD/LogP**	1.37
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=[N+]([O-])c1cccc(N)c1				
STD InChIKey	XJCVRTZCHMZPBD-UHFFFAOYAY				

Melting Points

mp °C	source
114.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
113.00	Alfa Aesar
114.00	PHYSPROP
112.50	Sigma-Aldrich

3-nitrobenzaldehyde C7H5NO3[2, 3, 64]



Compound Data

Melting point	**58.50 °C**	**331.65 K**			
CSID	7169	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	151.1195	**H bond donors**	0	**ACD/LogP**	1.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=[N+]([O-])c1cc(C=O)ccc1				
STD InChIKey	ZETIVVHRRQLWFW-UHFFFAOYAC				

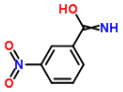
Melting Points

mp °C	source
59.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
58.00	Alfa Aesar

58.50	PHYSPROP

3-nitrobenzamide C7H6N2O3[3, 7, 64]

Compound Data



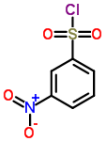
Melting point	**142.57 °C**	**415.72 K**			
CSID	11202219	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	166.1341	**H bond donors**	2	**ACD/LogP**	0.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.43 g/cm^3
SMILES	O=N(=O)c1cc(ccc1)C(=N)O				
STD InChIKey	KWAYEPXDGHYGRW-UHFFFAOYAE				

Melting Points

mp °C	source
142.00	Alfa Aesar
143.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
142.70	PHYSPROP

3-nitrobenzenesulfonyl chloride C6H4ClNO4S[3, 47]

Compound Data



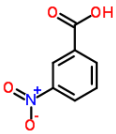
Melting point	**60.92 °C**	**334.07 K**			
CSID	8163	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	221.6183	**H bond donors**	0	**ACD/LogP**	2.21
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.61 g/cm^3
SMILES	O=S(Cl)(=O)c1cc([N+]([O-])=O)ccc1				
STD InChIKey	MWWNNNAOGWPTQY-UHFFFAOYAO				

Melting Points

mp °C	source
61.00	Alfa Aesar
60.85	IUCr

3-nitrobenzoic acid C7H5NO4[2, 3, 61, 64]

Compound Data



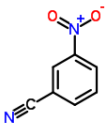
Melting point	**141.75 °C**	**414.90 K**			
CSID	8183	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	167.1189	**H bond donors**	1	**ACD/LogP**	1.82
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	O=[N+]([O-])c1cc(C(=O)O)ccc1				
STD InChIKey	AFPHTEQTJZKQAQ-UHFFFAOYAS				

Melting Points

mp °C	source
142.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
142.00	Alfa Aesar
142.00	Oxford University MSDS
141.00	PHYSPROP

3-nitrobenzonitrile C7H4N2O2[2, 3, 64]

Compound Data



Melting point	**116.33 °C**	**389.48 K**			
CSID	11582	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	148.1189	**H bond donors**	0	**ACD/LogP**	1.17
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.31 g/cm^3
SMILES	N#Cc1cccc([N+]([O-])=O)c1				
STD InChIKey	RUSAWEHOGCWOPG-UHFFFAOYAS				

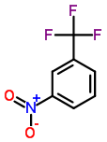
Melting Points

mp °C	source

117.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
116.00	Alfa Aesar
116.00	PHYSPROP

3-nitrobenzotrifluoride C7H4F3NO2[3, 64]

Compound Data



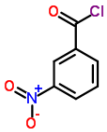
Melting point	**-3.70 °C**	**269.45 K**			
CSID	7108	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.1074	**H bond donors**	0	**ACD/LogP**	2.62
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.42 g/cm^3
SMILES	FC(F)(F)c1cccc([N+]([O-])=O)c1				
STD InChIKey	WHNAMGUAXHGCHH-UHFFFAOYAT				

Melting Points

mp °C	source
-5.00	Alfa Aesar
-2.40	PHYSPROP

3-nitrobenzoyl chloride C7H4ClNO3[3, 64]

Compound Data



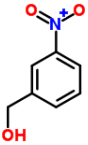
Melting point	**34.50 °C**	**307.65 K**			
CSID	8181	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	185.5646	**H bond donors**	0	**ACD/LogP**	2.12
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.45 g/cm^3
SMILES	O=[N+]([O-])c1cc(C(Cl)=O)ccc1				
STD InChIKey	NXTNASSYJUXJDV-UHFFFAOYAW				

Melting Points

mp °C	source
33.00	Alfa Aesar
36.00	PHYSPROP

3-nitrobenzyl alcohol C7H7NO3[2, 3, 64]

Compound Data



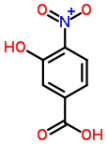
Melting point	**31.17 °C**	**304.32 K**			
CSID	62479	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	153.1354	**H bond donors**	1	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.33 g/cm^3
SMILES	[O-][N+](=O)c1cccc(c1)CO				
STD InChIKey	CWNPOQFCIIFQDM-UHFFFAOYAE				

Melting Points

mp °C	source
32.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
31.00	Alfa Aesar
30.50	PHYSPROP

3-nitrobenzyl alcohol C7H5NO5[3, 64]

Compound Data



Melting point	**232.00 °C**	**505.15 K**			
CSID	62477	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	183.1183	**H bond donors**	2	**ACD/LogP**	1.99
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.63 g/cm^3
SMILES	O=[N+]([O-])c1ccc(cc1O)C(=O)O				
STD InChIKey	XLDLRRGZWIEEHT-UHFFFAOYAO				

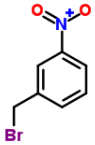
Melting Points

mp °C	source

234.00	Alfa Aesar
230.00	PHYSPROP

3-nitrobenzyl bromide C7H6BrNO2[2, 3, 64]

Compound Data



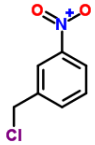
Melting point	**58.77 °C**	**331.92 K**			
CSID	69973	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	216.032	**H bond donors**	0	**ACD/LogP**	2.65
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.65 g/cm^3
SMILES	BrCc1cccc([N+]([O-])=O)c1				
STD InChIKey	LNWXALCHPJANMJ-UHFFFAOYAO				

Melting Points

mp °C	source
59.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
58.00	Alfa Aesar
59.30	PHYSPROP

3-nitrobenzyl chloride C7H6ClNO2[2, 3, 64]

Compound Data



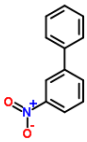
Melting point	**46.00 °C**	**319.15 K**			
CSID	11581	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	0	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	ClCc1cccc([N+]([O-])=O)c1				
STD InChIKey	APGGSERFJKEWFG-UHFFFAOYAI				

Melting Points

mp °C	source
47.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
45.00	Alfa Aesar
46.00	PHYSPROP

3-nitrobiphenyl C12H9NO2[3, 7, 64]

Compound Data



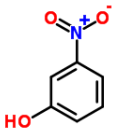
Melting point	**61.00 °C**	**334.15 K**			
CSID	15596	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	199.2054	**H bond donors**	0	**ACD/LogP**	3.51
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	[O-][N+](=O)c2cccc(c1ccccc1)c2				
STD InChIKey	FYRPEHRWMVMHQM-UHFFFAOYAM				

Melting Points

mp °C	source
59.00	Alfa Aesar
62.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
62.00	PHYSPROP

3-nitrophenol C6H5NO3[2, 3, 61, 64, 72, 72]

Compound Data

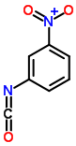


Melting point	**96.47 °C**	**369.62 K**			
CSID	10664	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	139.1088	**H bond donors**	1	**ACD/LogP**	1.93
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.40 g/cm^3
SMILES	O=[N+]([O-])c1cccc(O)c1				
STD InChIKey	RTZZCYNQPHTPPL-UHFFFAOYAM				

Melting Points

mp °C	source
98.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
96.00	Alfa Aesar
97.00	Oxford University MSDS
96.80	PHYSPROP
94.00	Sigma-Aldrich
97.00	Sigma-Aldrich

3-nitrophenyl isocyanate C7H4N2O3[3, 64]



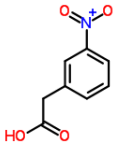
Compound Data

Melting point	**51.50 °C**	**324.65 K**			
CSID	69290	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	164.1183	**H bond donors**	0	**ACD/LogP**	2.49
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=C=N\c1cccc(c1)[N+]([O-])=O				
STD InChIKey	GFFGYTMCNVMFAJ-UHFFFAOYAM				

Melting Points

mp °C	source
52.00	Alfa Aesar
51.00	PHYSPROP

3-nitrophenylacetic acid C8H7NO4[3, 7, 64]



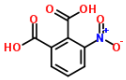
Compound Data

Melting point	**118.83 °C**	**391.98 K**			
CSID	15089	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	181.1455	**H bond donors**	1	**ACD/LogP**	1.24
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.41 g/cm^3
SMILES	O=C(O)Cc1cccc(c1)[N+]([O-])=O				
STD InChIKey	WUKHOVCMWXMOOA-UHFFFAOYAO				

Melting Points

mp °C	source
119.00	Alfa Aesar
119.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
118.50	PHYSPROP

3-nitrophthalic acid C8H5NO6[48, 61]



Compound Data

Melting point	**211.00 °C**	**484.15 K**			
CSID	62265	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	211.1284	**H bond donors**	2	**ACD/LogP**	0.67
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.67 g/cm^3
SMILES	O=[N+]([O-])c1cccc(c1C(=O)O)C(=O)O				
STD InChIKey	KFIRODWJCYBBHY-UHFFFAOYAC				

Melting Points

mp °C	source
212.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
210.00	Oxford University MSDS

3-nitrophthalimide C8H4N2O4[3, 64]

Compound Data

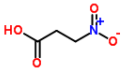
Melting point	**216.50 °C**	**489.65 K**			
CSID	11286	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	192.1284	**H bond donors**	1	**ACD/LogP**	0.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.61 g/cm^3

SMILES	[O-][N+](=O)c1cccc2c1C(=O)NC2=O
STD InChIKey	BONIIQYTWOPUQI-UHFFFAOYAD

Melting Points

mp °C	source
219.00	Alfa Aesar
214.00	PHYSPROP

3-nitropropanoic acid C3H5NO4[61, 64]



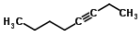
Compound Data

Melting point	**63.00 °C**	**336.15 K**			
CSID	1615	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	119.0761	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.39 g/cm^3
SMILES	C(C[N+](=O)[O-])C(=O)O				
STD InChIKey	WBLZUCOIBUDNBV-UHFFFAOYAZ				

Melting Points

mp °C	source
64.00	Oxford University MSDS
62.00	PHYSPROP

3-octyne C8H14[3, 4, 64]



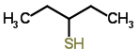
Compound Data

Melting point	**-103.97 °C**	**169.18 K**			
CSID	76541	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	3.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.77 g/cm^3
SMILES	C(#CCCCC)CC				
STD InChIKey	UDEISTCPVNLKRJ-UHFFFAOYAT				

Melting Points

mp °C	source
-104.00	Alfa Aesar
-104.00	American Petroleum Institute. Research Project 44; Selected ...
-103.90	PHYSPROP

3-pentanethiol C5H12S[4, 64]



Compound Data

Melting point	**-110.90 °C**	**162.25 K**			
CSID	62433	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	104.2138	**H bond donors**	0	**ACD/LogP**	2.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.83 g/cm^3
SMILES	SC(CC)CC				
STD InChIKey	WICKAMSPKJXSGN-UHFFFAOYAR				

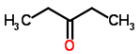
Melting Points

mp °C	source
-111.00	American Petroleum Institute. Research Project 44; Selected ...
-110.80	PHYSPROP

3-pentanone C5H10O[3, 4, 61, 64]

Compound Data

Melting point	**-39.25 °C**	**233.90 K**



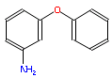
CSID	7016	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	86.1323	**H bond donors**	0	**ACD/LogP**	0.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.80 g/cm^3
SMILES	O=C(CC)CC				
STD InChIKey	FDPIMTJIUBPUKL-UHFFFAOYAJ				

Melting Points

mp °C	source
-39.00	Alfa Aesar
-39.00	American Petroleum Institute. Research Project 44; Selected ...
-40.00	Oxford University MSDS
-39.00	PHYSPROP

3-phenoxyaniline C12H11NO[3, 64]

Compound Data



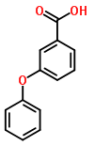
Melting point	**36.50 °C**	**309.65 K**			
CSID	21170956	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	185.2218	**H bond donors**	2	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	Nc2cccc(Oc1ccccc1)c2				
STD InChIKey	UCSYVYFGMFODMY-UHFFFAOYAB				

Melting Points

mp °C	source
36.00	Alfa Aesar
37.00	PHYSPROP

3-phenoxybenzoic acid C13H10O3[3, 64]

Compound Data



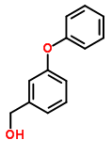
Melting point	**148.75 °C**	**421.90 K**			
CSID	18409	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.2167	**H bond donors**	1	**ACD/LogP**	3.91
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.24 g/cm^3
SMILES	O=C(O)c2cc(Oc1ccccc1)ccc2				
STD InChIKey	NXTDJHZGHOFSQG-UHFFFAOYAC				

Melting Points

mp °C	source
148.00	Alfa Aesar
149.50	PHYSPROP

3-phenoxybenzyl alcohol C13H12O2[3, 61]

Compound Data



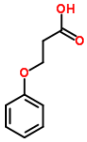
Melting point	**8.00 °C**	**281.15 K**			
CSID	24499	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.2332	**H bond donors**	1	**ACD/LogP**	3.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.15 g/cm^3
SMILES	O(c1ccccc1)c2cc(ccc2)CO				
STD InChIKey	KGANAERDZBAECK-UHFFFAOYAU				

Melting Points

mp °C	source
6.00	Alfa Aesar
10.00	Oxford University MSDS

3-phenoxypropionic acid C9H10O3[3, 64]

Compound Data



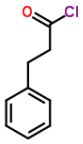
Melting point	**97.75 °C**	**370.90 K**			
CSID	73626	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	1.63
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(O)CCOc1ccccc1				
STD InChIKey	BUSOTUQRURCMCM-UHFFFAOYAR				

Melting Points

mp °C	source
98.00	Alfa Aesar
97.50	PHYSPROP

3-phenylpropionyl chloride C9H9ClO[3, 64]

Compound Data



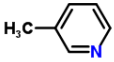
Melting point	**-4.50 °C**	**268.65 K**			
CSID	58333	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	168.6202	**H bond donors**	0	**ACD/LogP**	2.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	ClC(=O)CCc1ccccc1				
STD InChIKey	MFEILWXBDBCWKF-UHFFFAOYAM				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-2.00	PHYSPROP

3-picoline C6H7N[3, 32, 64]

Compound Data



Melting point	**-18.07 °C**	**255.08 K**			
CSID	21106520	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	93.1265	**H bond donors**	0	**ACD/LogP**	1.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.94 g/cm^3
SMILES	Cc1cccnc1				
STD InChIKey	ITQTTZVARXURQS-UHFFFAOYAH				

Melting Points

mp °C	source
-18.00	Alfa Aesar
-18.10	DrugBank
-18.10	PHYSPROP

3-picoline n-oxide C6H7NO[3, 64]

Compound Data

Melting point	**38.50 °C**	**311.65 K**			
CSID	13258	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	0	**ACD/LogP**	-0.74
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.01 g/cm^3
SMILES	[O-][n+]1cccc(c1)C				
STD InChIKey	DMGGLIWGZFZLIY-UHFFFAOYAT				

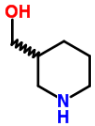
Melting Points

mp °C	source
38.00	Alfa Aesar
39.00	PHYSPROP

3-piperidinemethanol C6H13NO[3, 64]

Compound Data

Melting point	**60.50 °C**	**333.65 K**



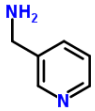
CSID	96573	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	115.1735	**H bond donors**	2	**ACD/LogP**	-0.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.95 g/cm^3
SMILES	OCC1CCCNC1				
STD InChIKey	VUNPWIPIOOMCPT-UHFFFAOYAZ				

Melting Points

mp °C	source
60.00	Alfa Aesar
61.00	PHYSPROP

3-pyridylmethylamine C6H8N2[3, 64]

Compound Data



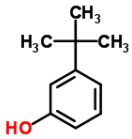
Melting point	**-21.05 °C**	**252.10 K**			
CSID	28777	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	2	**ACD/LogP**	-0.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	n1cccc(c1)CN				
STD InChIKey	HDOUGSFASVGDCS-UHFFFAOYAI				

Melting Points

mp °C	source
-21.00	Alfa Aesar
-21.10	PHYSPROP

3-t-butylphenol C10H14O[3, 31, 64]

Compound Data



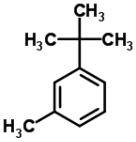
Melting point	**42.77 °C**	**315.92 K**			
CSID	10966	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	1	**ACD/LogP**	3.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	Oc1cc(ccc1)C(C)(C)C				
STD InChIKey	CYEKUDPFXBLGHH-UHFFFAOYAF				

Melting Points

mp °C	source
45.00	Alfa Aesar
41.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
42.30	PHYSPROP

3-t-butyltoluene C11H16[3, 4, 64]

Compound Data



Melting point	**-41.13 °C**	**232.02 K**			
CSID	31082	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	148.2447	**H bond donors**	0	**ACD/LogP**	4.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.86 g/cm^3
SMILES	c1ccc(cc1C(C)(C)C)C				
STD InChIKey	JTIAYWZZZOZUTK-UHFFFAOYAW				

Melting Points

mp °C	source
-41.00	Alfa Aesar
-41.00	American Petroleum Institute. Research Project 44; Selected ...
-41.40	PHYSPROP

3-thiaheptane C6H14S[4, 64]

Compound Data

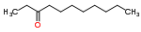
Melting point	**-95.05 °C**	**178.10 K**			
CSID	12011	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.2404	**H bond donors**	0	**ACD/LogP**	3.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.83 g/cm^3
SMILES	S(CC)CCCC				
STD InChIKey	XJIRSLHMKBUGMR-UHFFFAOYAK				

Melting Points

mp °C	source
-95.00	American Petroleum Institute. Research Project 44; Selected ...
-95.10	PHYSPROP

3-undecanone C11H22O[2, 3, 64]

Compound Data



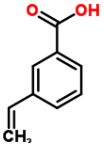
Melting point	**11.33 °C**	**284.48 K**			
CSID	67735	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2918	**H bond donors**	0	**ACD/LogP**	4.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.82 g/cm^3
SMILES	O=C(CCCCCCCC)CC				
STD InChIKey	YNMZZHPSYMOGCI-UHFFFAOYAM				

Melting Points

mp °C	source
13.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
9.00	Alfa Aesar
12.00	PHYSPROP

3-vinylbenzoic acid C9H8O2[3, 7]

Compound Data



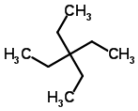
Melting point	**95.50 °C**	**368.65 K**			
CSID	3637837	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	148.1586	**H bond donors**	1	**ACD/LogP**	2.38
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.16 g/cm^3
SMILES	O=C(O)c1cccc(\C=C)c1				
STD InChIKey	VWXZFDWVWMQRQR-UHFFFAOYAJ				

Melting Points

mp °C	source
95.00	Alfa Aesar
96.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

3,3-diethylpentane C9H20[4, 64]

Compound Data



Melting point	**-33.05 °C**	**240.10 K**			
CSID	13402	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	5.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.72 g/cm^3
SMILES	CCC(CC)(CC)CC				
STD InChIKey	BGXXXYLRPIRDHJ-UHFFFAOYAE				

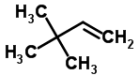
Melting Points

mp °C	source
-33.00	American Petroleum Institute. Research Project 44; Selected ...
-33.10	PHYSPROP

3,3-dimethyl-1-butene C6H12[3, 4, 64]

Compound Data

Melting point	**-115.07 °C**	**158.08 K**



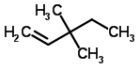
CSID	10737	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.07
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.69 g/cm^3
SMILES	C=C\C(C)(C)C				
STD InChIKey	PKXHXOTZMFCXSH-UHFFFAOYAA				

Melting Points

mp °C	source
-115.00	Alfa Aesar
-115.00	American Petroleum Institute. Research Project 44; Selected ...
-115.20	PHYSPROP

3,3-dimethyl-1-pentene C7H14[4, 64]

Compound Data



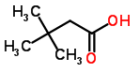
Melting point	**-134.15 °C**	**139.00 K**			
CSID	17801	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.70 g/cm^3
SMILES	C=C\C(C)(C)CC				
STD InChIKey	TXBZITDWMURSEF-UHFFFAOYAV				

Melting Points

mp °C	source
-134.00	American Petroleum Institute. Research Project 44; Selected ...
-134.30	PHYSPROP

3,3-dimethylbutyric acid C6H12O2[3, 64]

Compound Data



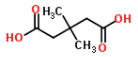
Melting point	**6.25 °C**	**279.40 K**			
CSID	13438	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	1	**ACD/LogP**	1.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.95 g/cm^3
SMILES	O=C(O)CC(C)(C)C				
STD InChIKey	MLMQPDHYNJCQAO-UHFFFAOYAR				

Melting Points

mp °C	source
6.00	Alfa Aesar
6.50	PHYSPROP

3,3-dimethylglutaric acid C7H12O4[3, 64]

Compound Data



Melting point	**102.25 °C**	**375.40 K**			
CSID	19739	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	160.1678	**H bond donors**	2	**ACD/LogP**	-0.34
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	O=C(O)CC(C)(CC(=O)O)C				
STD InChIKey	DUHQIGLHYXLKAE-UHFFFAOYAV				

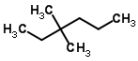
Melting Points

mp °C	source
101.00	Alfa Aesar
103.50	PHYSPROP

3,3-dimethylhexane C8H18[4, 64]

Compound Data

Melting point	**-126.05 °C**	**147.10 K**



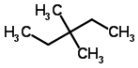
CSID	10759	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	4.64
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.71 g/cm^3
SMILES	CC(C)(CC)CCC				
STD InChIKey	KUMXLFIBWFCMOJ-UHFFFAOYAZ				

Melting Points

mp °C	source
-126.00	American Petroleum Institute. Research Project 44; Selected ...
-126.10	PHYSPROP

3,3-dimethylpentane C7H16[3, 4, 64]

Compound Data



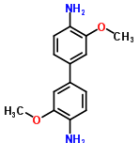
Melting point	**-134.63 °C**	**138.52 K**			
CSID	10755	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.2019	**H bond donors**	0	**ACD/LogP**	4.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.69 g/cm^3
SMILES	CC(C)(CC)CC				
STD InChIKey	AEXMKKGTQYQZCS-UHFFFAOYAS				

Melting Points

mp °C	source
-135.00	Alfa Aesar
-134.00	American Petroleum Institute. Research Project 44; Selected ...
-134.90	PHYSPROP

3,3'-dimethoxybiphenyl-4,4'-diamine C14H16N2O2[3, 64]

Compound Data



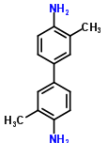
Melting point	**136.50 °C**	**409.65 K**			
CSID	8104	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	244.289	**H bond donors**	4	**ACD/LogP**	1.57
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.18 g/cm^3
SMILES	O(c1cc(ccc1N)c2ccc(N)c(OC)c2)C				
STD InChIKey	JRBJSXQPQWSCCF-UHFFFAOYAM				

Melting Points

mp °C	source
136.00	Alfa Aesar
137.00	PHYSPROP

3,3'-dimethyl-4,4'-biphenyldiamine C14H16N2[3, 64]

Compound Data



Melting point	**130.75 °C**	**403.90 K**			
CSID	8106	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2902	**H bond donors**	4	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	c2(c1ccc(N)c(c1)C)ccc(N)c(c2)C				
STD InChIKey	NUIURNJTPRWVAP-UHFFFAOYAK				

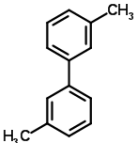
Melting Points

mp °C	source
130.00	Alfa Aesar
131.50	PHYSPROP

3,3'-dimethylbiphenyl C14H14[4, 64]

Compound Data

Melting point	**8.00 °C**	**281.15 K**



CSID	11437	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	c2c(c1cccc(c1)C)cccc2C				
STD InChIKey	GVEDOIATHPCYGS-UHFFFAOYAW				

Melting Points

mp °C	source
7.00	American Petroleum Institute. Research Project 44; Selected ...
9.00	PHYSPROP

3,4-diaminopyridine C5H7N3[3, 64, 64, 72]

Compound Data

Melting point	**218.50 °C**	**491.65 K**			
CSID	5705	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	109.1292	**H bond donors**	4	**ACD/LogP**	-0.09
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	c1cncc(c1N)N				
STD InChIKey	OYTKINVCDFNREN-UHFFFAOYAR				

Melting Points

mp °C	source
219.00	Alfa Aesar
220.00	PHYSPROP
216.50	Sigma-Aldrich
	Values not used in calculating the average melting point
120.80	PHYSPROP[1]

1. clearly out of range JCB

3,4-dibromothiophene C4H2Br2S[3, 64]

Compound Data

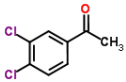
Melting point	**4.75 °C**	**277.90 K**			
CSID	17428	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	241.9317	**H bond donors**	0	**ACD/LogP**	3.21
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.17 g/cm^3
SMILES	Brc1scc1Br				
STD InChIKey	VGKLVWTVCUDISO-UHFFFAOYAN				

Melting Points

mp °C	source
5.00	Alfa Aesar
4.50	PHYSPROP

3,4-dichloroacetophenone C8H6Cl2O[2, 3, 64]

Compound Data

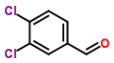


Melting point	**74.33 °C**	**347.48 K**			
CSID	68350	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	189.0386	**H bond donors**	0	**ACD/LogP**	3.06
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	CC(=O)c1ccc(c(c1)Cl)Cl				
STD InChIKey	WBPAOUHWPONFEQ-UHFFFAOYAT				

Melting Points

mp °C	source
73.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
74.00	Alfa Aesar
76.00	PHYSPROP

3,4-dichlorobenzaldehyde C7H4Cl2O[2, 3, 64]



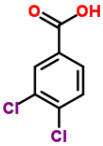
Compound Data

Melting point	**43.67 °C**	**316.82 K**			
CSID	21106577	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.0121	**H bond donors**	0	**ACD/LogP**	2.70
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Clc1ccc(C=O)cc1Cl				
STD InChIKey	ZWUSBSHBFFPRNE-UHFFFAOYAS				

Melting Points

mp °C	source
44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
43.00	Alfa Aesar
44.00	PHYSPROP

3,4-dichlorobenzoic acid C7H4Cl2O2[2, 3]



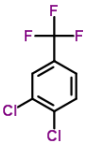
Compound Data

Melting point	**207.50 °C**	**480.65 K**			
CSID	5612	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	191.0115	**H bond donors**	1	**ACD/LogP**	3.53
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	Clc1ccc(C(=O)O)cc1Cl				
STD InChIKey	VPHHJAOJUJHJKD-UHFFFAOYAX				

Melting Points

mp °C	source
208.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
207.00	Alfa Aesar

3,4-dichlorobenzotrifluoride C7H3Cl2F3[3, 64]



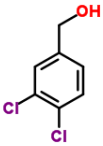
Compound Data

Melting point	**-12.25 °C**	**260.90 K**			
CSID	9109	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	214.9999	**H bond donors**	0	**ACD/LogP**	4.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.46 g/cm^3
SMILES	Clc1ccc(cc1Cl)C(F)(F)F				
STD InChIKey	XILPLWOGHPSJBK-UHFFFAOYAR				

Melting Points

mp °C	source
-12.00	Alfa Aesar
-12.50	PHYSPROP

3,4-dichlorobenzyl alcohol C7H6Cl2O[3, 64]



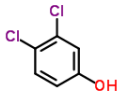
Compound Data

Melting point	**37.00 °C**	**310.15 K**			
CSID	14956	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	Clc1ccc(cc1Cl)CO				
STD InChIKey	FVJIUQSKXOYFKG-UHFFFAOYAY				

Melting Points

mp °C	source
38.00	Alfa Aesar
36.00	PHYSPROP

3,4-dichlorophenol C6H4Cl2O[2, 3, 28, 61, 64, 72]



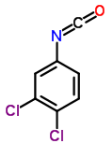
Compound Data

Melting point	**67.00 °C**	**340.15 K**			
CSID	6988	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.0014	**H bond donors**	1	**ACD/LogP**	3.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	Clc1ccc(O)cc1Cl				
STD InChIKey	WDNBURPWRNALGP-UHFFFAOYAE				

Melting Points

mp °C	source
67.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
66.00	Alfa Aesar
68.00	CRC Handbook of Chemistry and Physics
67.00	Oxford University MSDS
68.00	PHYSPROP
66.00	Sigma-Aldrich

3,4-dichlorophenyl isocyanate C7H3Cl2NO[3, 64]



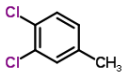
Compound Data

Melting point	**42.50 °C**	**315.65 K**			
CSID	7325	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	188.0108	**H bond donors**	0	**ACD/LogP**	4.01
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	Clc1ccc(/N=C=O)cc1Cl				
STD InChIKey	MFUVCHZWGSJKEQ-UHFFFAOYAC				

Melting Points

mp °C	source
42.00	Alfa Aesar
43.00	PHYSPROP

3,4-dichlorotoluene C7H6Cl2[3, 31, 64]



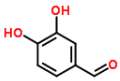
Compound Data

Melting point	**-15.07 °C**	**258.08 K**			
CSID	21106517	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	161.0285	**H bond donors**	0	**ACD/LogP**	3.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	Cc1cc(Cl)c(Cl)cc1				
STD InChIKey	WYUIWKFIFOJVKW-UHFFFAOYAF				

Melting Points

mp °C	source
-15.00	Alfa Aesar
-15.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-15.20	PHYSPROP

3,4-dihydroxybenzaldehyde C7H6O3[2, 3, 61]



Compound Data

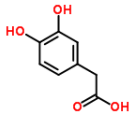
Melting point	**154.00 °C**	**427.15 K**			
CSID	8438	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	138.1207	**H bond donors**	2	**ACD/LogP**	1.14
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.41 g/cm^3
SMILES	O=Cc1cc(O)c(O)cc1				
STD InChIKey	IBGBGRVKPALMCQ-UHFFFAOYAN				

Melting Points

mp °C	source
153.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
155.00	Alfa Aesar

154.00	Oxford University MSDS

3,4-dihydroxyphenylacetic acid C8H8O4[3, 32, 64]



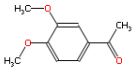
Compound Data

Melting point	**128.67 °C**	**401.82 K**			
CSID	532	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	3	**ACD/LogP**	0.17
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.48 g/cm^3
SMILES	O=C(O)Cc1cc(O)c(O)cc1				
STD InChIKey	CFFZDZCDUFSOFZ-UHFFFAOYAU				

Melting Points

mp °C	source
129.00	Alfa Aesar
128.50	DrugBank
128.50	PHYSPROP

3,4-dimethoxyacetophenone C10H12O3[2, 3, 64]



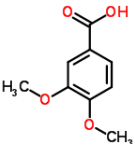
Compound Data

Melting point	**50.33 °C**	**323.48 K**			
CSID	21168556	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	0	**ACD/LogP**	1.82
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	COc1cc(ccc1OC)C(C)=O				
STD InChIKey	IQZLUWLMQNGTIW-UHFFFAOYAO				

Melting Points

mp °C	source
51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
49.00	Alfa Aesar
51.00	PHYSPROP

3,4-dimethoxybenzoic acid C9H10O4[3, 61, 64, 64]



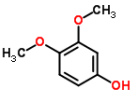
Compound Data

Melting point	**180.50 °C**	**453.65 K**			
CSID	6854	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.1733	**H bond donors**	1	**ACD/LogP**	1.39
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	COc1ccc(cc1OC)C(=O)O				
STD InChIKey	DAUAQNGYDSHRET-UHFFFAOYAJ				

Melting Points

mp °C	source
181.00	Alfa Aesar
180.00	Oxford University MSDS
181.00	PHYSPROP
180.00	PHYSPROP

3,4-dimethoxyphenol C8H10O3[2, 3]



Compound Data

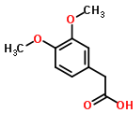
Melting point	**82.00 °C**	**355.15 K**			
CSID	15420	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	154.1632	**H bond donors**	1	**ACD/LogP**	1.25
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.13 g/cm^3
SMILES	O(c1ccc(O)cc1OC)C				
STD InChIKey	SMFFZOQLHYIRDA-UHFFFAOYAA				

Melting Points

mp °C	source
83.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
81.00	Alfa Aesar

3,4-dimethoxyphenylacetic acid C10H12O4[3, 61]

Compound Data



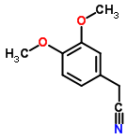
Melting point	**97.50 °C**	**370.65 K**			
CSID	6872	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	196.1999	**H bond donors**	1	**ACD/LogP**	1.24
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.19 g/cm^3
SMILES	O=C(O)Cc1cc(OC)c(OC)cc1				
STD InChIKey	WUAXWQRULBZETB-UHFFFAOYAW				

Melting Points

mp °C	source
97.00	Alfa Aesar
98.00	Oxford University MSDS

3,4-dimethoxyphenylacetonitrile C10H11NO2[3, 64]

Compound Data



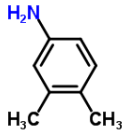
Melting point	**63.38 °C**	**336.52 K**			
CSID	60093	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	177.1998	**H bond donors**	0	**ACD/LogP**	1.19
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	N#CCc1cc(OC)c(OC)cc1				
STD InChIKey	ASLSUMISAQDOOB-UHFFFAOYAS				

Melting Points

mp °C	source
64.00	Alfa Aesar
62.75	PHYSPROP

3,4-dimethylaniline C8H11N[2, 3, 64]

Compound Data



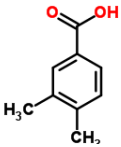
Melting point	**50.67 °C**	**323.82 K**			
CSID	13860491	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	Cc1cc(N)ccc1C				
STD InChIKey	DOLQYFPDPKPQSS-UHFFFAOYAG				

Melting Points

mp °C	source
51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
50.00	Alfa Aesar
51.00	PHYSPROP

3,4-dimethylbenzoic acid C9H10O2[3, 64]

Compound Data



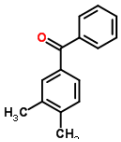
Melting point	**165.50 °C**	**438.65 K**			
CSID	11576	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	2.81
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	O=C(O)c1cc(c(cc1)C)C				
STD InChIKey	OPVAJFQBSDUNQA-UHFFFAOYAK				

Melting Points

mp °C	source

166.00	Alfa Aesar
165.00	PHYSPROP

3,4-dimethylbenzophenone C15H14O[3, 64]



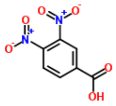
Compound Data

Melting point	**46.75 °C**	**319.90 K**			
CSID	68247	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	210.2711	**H bond donors**	0	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	O=C(c1cc(c(cc1)C)C)c2ccccc2				
STD InChIKey	JENOLWCGNVWTJN-UHFFFAOYAX				

Melting Points

mp °C	source
46.00	Alfa Aesar
47.50	PHYSPROP

3,4-dinitrobenzoic acid C7H4N2O6[3, 64]



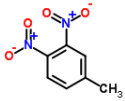
Compound Data

Melting point	**165.50 °C**	**438.65 K**			
CSID	10259	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	212.1165	**H bond donors**	1	**ACD/LogP**	1.98
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.69 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1[N+]([O-])=O)C(=O)O				
STD InChIKey	OMVRRHJJQILIJX-UHFFFAOYAQ				

Melting Points

mp °C	source
165.00	Alfa Aesar
166.00	PHYSPROP

3,4-dinitrotoluene C7H6N2O4[2, 3, 64]



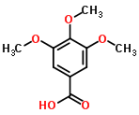
Compound Data

Melting point	**56.77 °C**	**329.92 K**			
CSID	11390	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	182.1335	**H bond donors**	0	**ACD/LogP**	2.30
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	O=[N+]([O-])c1c(ccc(c1)C)[N+]([O-])=O				
STD InChIKey	INYDMNPNDHRJQJ-UHFFFAOYAV				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
56.00	Alfa Aesar
58.30	PHYSPROP

3,4,5-trimethoxybenzoic acid C10H12O5[3, 48, 64]



Compound Data

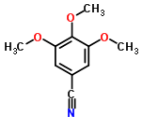
Melting point	**171.43 °C**	**444.58 K**			
CSID	8054	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	212.1993	**H bond donors**	1	**ACD/LogP**	1.90
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.22 g/cm^3
SMILES	O=C(O)c1cc(OC)c(OC)c(OC)c1				
STD InChIKey	SJSOFNCYXJUNBT-UHFFFAOYAD				

Melting Points

mp °C	source
170.00	Alfa Aesar

172.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
172.30	PHYSPROP

3,4,5-trimethoxybenzonitrile C10H11NO3[3, 48, 64]



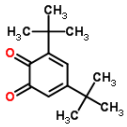
Compound Data

Melting point	**93.60 °C**	**366.75 K**			
CSID	15105	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	193.1992	**H bond donors**	0	**ACD/LogP**	1.15
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	N#Cc1cc(OC)c(OC)c(OC)c1				
STD InChIKey	OSBQUSPVORCDCU-UHFFFAOYAQ				

Melting Points

mp °C	source
93.00	Alfa Aesar
94.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
93.80	PHYSPROP

3,5-di-t-butyl-1,2-benzoquinone C14H20O2[3, 61]



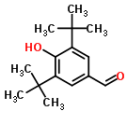
Compound Data

Melting point	**114.25 °C**	**387.40 K**			
CSID	69366	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	220.3074	**H bond donors**	0	**ACD/LogP**	3.04
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	O=C1/C(=C\C(=C/C1=O)C(C)(C)C)C(C)(C)C				
STD InChIKey	NOUZOVBGCDDMSX-UHFFFAOYAY				

Melting Points

mp °C	source
115.00	Alfa Aesar
113.50	Oxford University MSDS

3,5-di-t-butyl-4-hydroxybenzaldehyde C15H22O2[3, 64]



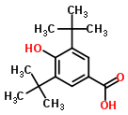
Compound Data

Melting point	**187.00 °C**	**460.15 K**			
CSID	65974	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	234.334	**H bond donors**	1	**ACD/LogP**	4.77
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.01 g/cm^3
SMILES	O=Cc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C				
STD InChIKey	DOZRDZLFLOODMB-UHFFFAOYAD				

Melting Points

mp °C	source
188.00	Alfa Aesar
186.00	PHYSPROP

3,5-di-t-butyl-4-hydroxybenzoic acid C15H22O3[3, 64]



Compound Data

Melting point	**207.75 °C**	**480.90 K**			
CSID	14285	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	250.3334	**H bond donors**	2	**ACD/LogP**	4.80
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.07 g/cm^3
SMILES	O=C(O)c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C				
STD InChIKey	YEXOWHQZWLCHHD-UHFFFAOYAK				

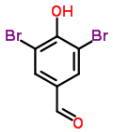
Melting Points

mp °C	source
208.00	Alfa Aesar

207.50	PHYSPROP

3,5-dibromo-4-hydroxybenzaldehyde C7H4Br2O2[3, 48]

Compound Data



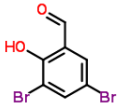
Melting point	**181.50 °C**	**454.65 K**			
CSID	17097	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	279.9135	**H bond donors**	1	**ACD/LogP**	3.53
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.12 g/cm^3
SMILES	Brc1cc(cc(Br)c1O)C=O				
STD InChIKey	SXRHGLQCOLNZPT-UHFFFAOYAU				

Melting Points

mp °C	source
181.00	Alfa Aesar
182.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

3,5-dibromosalicylaldehyde C7H4Br2O2[3, 64]

Compound Data



Melting point	**84.50 °C**	**357.65 K**			
CSID	6757	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	279.9135	**H bond donors**	1	**ACD/LogP**	3.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.12 g/cm^3
SMILES	Brc1cc(Br)cc(C=O)c1O				
STD InChIKey	JHZOXYGFQMROFJ-UHFFFAOYAH				

Melting Points

mp °C	source
83.00	Alfa Aesar
86.00	PHYSPROP

3,5-dibromosalicylic acid C7H4Br2O3[3, 64]

Compound Data

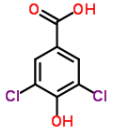
Melting point	**227.00 °C**	**500.15 K**			
CSID	17440	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	295.9129	**H bond donors**	2	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.23 g/cm^3
SMILES	Brc1cc(Br)cc(C(=O)O)c1O				
STD InChIKey	BFBZHSOXKROMBG-UHFFFAOYAZ				

Melting Points

mp °C	source
226.00	Alfa Aesar
228.00	PHYSPROP

3,5-dichloro-4-hydroxybenzoic acid C7H4Cl2O3[3, 64]

Compound Data

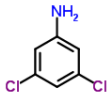


Melting point	**266.50 °C**	**539.65 K**			
CSID	17704	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	207.0109	**H bond donors**	2	**ACD/LogP**	3.37
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.67 g/cm^3
SMILES	Clc1cc(cc(Cl)c1O)C(=O)O				
STD InChIKey	AULKDLUOQCUNOK-UHFFFAOYAH				

Melting Points

mp °C	source
268.00	Alfa Aesar
265.00	PHYSPROP

3,5-dichloroaniline C6H5Cl2N[2, 3, 64]



Compound Data

Melting point	**52.00 °C**	**325.15 K**			
CSID	11778	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.0166	**H bond donors**	2	**ACD/LogP**	2.70
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Clc1cc(N)cc(Cl)c1				
STD InChIKey	UQRLKWGPEVNVHT-UHFFFAOYAN				

Melting Points

mp °C	source
53.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
51.00	Alfa Aesar
52.00	PHYSPROP

3,5-dichloroanisole C7H6Cl2O[2, 3, 64]

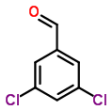
Compound Data

Melting point	**40.67 °C**	**313.82 K**			
CSID	33621	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	0	**ACD/LogP**	3.80
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Clc1cc(OC)cc(Cl)c1				
STD InChIKey	SSNXYMVLSOMJLU-UHFFFAOYAF				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
41.00	Alfa Aesar
41.00	PHYSPROP

3,5-dichlorobenzaldehyde C7H4Cl2O[3, 48, 64]



Compound Data

Melting point	**65.33 °C**	**338.48 K**			
CSID	32882	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.0121	**H bond donors**	0	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	Clc1cc(C=O)cc(Cl)c1				
STD InChIKey	CASRSOJWLARCRX-UHFFFAOYAT				

Melting Points

mp °C	source
63.00	Alfa Aesar
68.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
65.00	PHYSPROP

3,5-dichlorobenzoic acid C7H4Cl2O2[2, 3, 64]

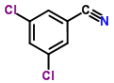
Compound Data

Melting point	**186.67 °C**	**459.82 K**			
CSID	5606	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	191.0115	**H bond donors**	1	**ACD/LogP**	3.92
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	Clc1cc(C(=O)O)cc(Cl)c1				
STD InChIKey	CXKCZFDUOYMOOP-UHFFFAOYAI				

Melting Points

mp °C	source
186.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
186.00	Alfa Aesar
188.00	PHYSPROP

3,5-dichlorobenzonitrile C7H3Cl2N[2, 3]



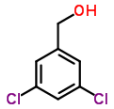
Compound Data

Melting point	**65.00 °C**	**338.15 K**			
CSID	73125	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	172.0114	**H bond donors**	0	**ACD/LogP**	2.69
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	c1c(cc(cc1Cl)Cl)C#N				
STD InChIKey	PUJSUOGJGIECFQ-UHFFFAOYAP				

Melting Points

mp °C	source
64.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
66.00	Alfa Aesar

3,5-dichlorobenzyl alcohol C7H6Cl2O[3, 64]



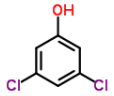
Compound Data

Melting point	**79.25 °C**	**352.40 K**			
CSID	39404	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	177.0279	**H bond donors**	1	**ACD/LogP**	2.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	Clc1cc(cc(Cl)c1)CO				
STD InChIKey	VSNNLLQKDRCKCB-UHFFFAOYAF				

Melting Points

mp °C	source
78.00	Alfa Aesar
80.50	PHYSPROP

3,5-dichlorophenol C6H4Cl2O[2, 3, 64]



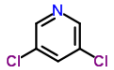
Compound Data

Melting point	**67.33 °C**	**340.48 K**			
CSID	11083	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	163.0014	**H bond donors**	1	**ACD/LogP**	3.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	Clc1cc(O)cc(Cl)c1				
STD InChIKey	VPOMSPZBQMDLTM-UHFFFAOYAL				

Melting Points

mp °C	source
68.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
66.00	Alfa Aesar
68.00	PHYSPROP

3,5-dichloropyridine C5H3Cl2N[3, 64]



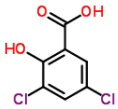
Compound Data

Melting point	**65.50 °C**	**338.65 K**			
CSID	16237	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	147.99	**H bond donors**	0	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	Clc1cncc(Cl)c1				
STD InChIKey	WPGHPGAUFIJVJF-UHFFFAOYAF				

Melting Points

mp °C	source
65.00	Alfa Aesar
66.00	PHYSPROP

3,5-dichlorosalicylic acid C7H4Cl2O3[3, 64]



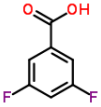
Compound Data

Melting point	**222.25 °C**	**495.40 K**			
CSID	9073	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	207.0109	**H bond donors**	2	**ACD/LogP**	4.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.67 g/cm^3
SMILES	Clc1cc(Cl)cc(C(=O)O)c1O				
STD InChIKey	CNJGWCQEGROXEE-UHFFFAOYAB				

Melting Points

mp °C	source
224.00	Alfa Aesar
220.50	PHYSPROP

3,5-difluorobenzoic acid C7H4F2O2[3, 64]



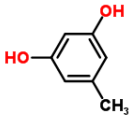
Compound Data

Melting point	**121.50 °C**	**394.65 K**			
CSID	91500	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1023	**H bond donors**	1	**ACD/LogP**	2.47
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.43 g/cm^3
SMILES	Fc1cc(C(=O)O)cc(F)c1				
STD InChIKey	GONAVIHGXFBTOZ-UHFFFAOYAZ				

Melting Points

mp °C	source
121.00	Alfa Aesar
122.00	PHYSPROP

3,5-dihydroxytoluene C7H8O2[3, 64]



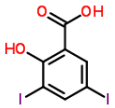
Compound Data

Melting point	**107.25 °C**	**380.40 K**			
CSID	13839080	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	1.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	Cc1cc(O)cc(O)c1				
STD InChIKey	OIPPWFOQEKKFEE-UHFFFAOYAN				

Melting Points

mp °C	source
107.00	Alfa Aesar
107.50	PHYSPROP

3,5-diiodosalicylic acid C7H4I2O3[3, 64]



Compound Data

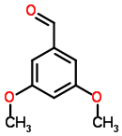
Melting point	**233.25 °C**	**506.40 K**			
CSID	8310	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	389.9138	**H bond donors**	2	**ACD/LogP**	4.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.70 g/cm^3
SMILES	Ic1cc(C(=O)O)c(O)c(I)c1				
STD InChIKey	DHZVWQPHNWDCFS-UHFFFAOYAS				

Melting Points

mp °C	source
231.00	Alfa Aesar
235.50	PHYSPROP

3,5-dimethoxybenzaldehyde C9H10O3[2, 3, 35, 64]

Compound Data



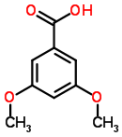
Melting point	**46.40 °C**	**319.55 K**			
CSID	73763	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	0	**ACD/LogP**	1.53
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=Cc1cc(OC)cc(OC)c1				
STD InChIKey	VFZRZRDOXPRTSC-UHFFFAOYAG				

Melting Points

mp °C	source
47.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
46.00	Alfa Aesar
46.30	EPISuite-ChemSpider
46.30	PHYSPROP

3,5-dimethoxybenzoic acid C9H10O4[3, 64]

Compound Data



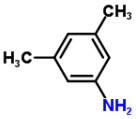
Melting point	**184.75 °C**	**457.90 K**			
CSID	13693	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.1733	**H bond donors**	1	**ACD/LogP**	2.03
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	O=C(O)c1cc(OC)cc(OC)c1				
STD InChIKey	IWPZKOJSYQZABD-UHFFFAOYAJ				

Melting Points

mp °C	source
184.00	Alfa Aesar
185.50	PHYSPROP

3,5-dimethylaniline C8H11N[3, 64]

Compound Data



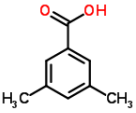
Melting point	**9.90 °C**	**283.05 K**			
CSID	21106578	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	Cc1cc(N)cc(C)c1				
STD InChIKey	MKARNSWMMBGSHX-UHFFFAOYAO				

Melting Points

mp °C	source
10.00	Alfa Aesar
9.80	PHYSPROP

3,5-dimethylbenzoic acid C9H10O2[3, 64]

Compound Data



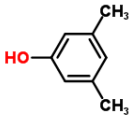
Melting point	**170.55 °C**	**443.70 K**			
CSID	9929	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	2.81
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	O=C(O)c1cc(cc(c1)C)C				
STD InChIKey	UMVOQQDNEYOJOK-UHFFFAOYAD				

Melting Points

mp °C	source
170.00	Alfa Aesar
171.10	PHYSPROP

3,5-dimethylphenol C8H10O[3, 28, 64, 72, 72]

Compound Data



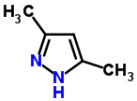
Melting point	**63.60 °C**	**336.75 K**			
CSID	13839110	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	Cc1cc(O)cc(C)c1				
STD InChIKey	TUAMRELNJMMDMT-UHFFFAOYAS				

Melting Points

mp °C	source
63.00	Alfa Aesar
63.40	CRC Handbook of Chemistry and Physics
63.60	PHYSPROP
62.50	Sigma-Aldrich
65.50	Sigma-Aldrich

3,5-dimethylpyrazole C5H8N2[3, 64]

Compound Data



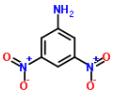
Melting point	**107.25 °C**	**380.40 K**			
CSID	5975	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	96.1304	**H bond donors**	1	**ACD/LogP**	1.24
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.03 g/cm^3
SMILES	n1c(cc(n1)C)C				
STD InChIKey	SDXAWLJRERMRKF-UHFFFAOYAF				

Melting Points

mp °C	source
107.00	Alfa Aesar
107.50	PHYSPROP

3,5-dinitroaniline C6H5N3O4[2, 64]

Compound Data



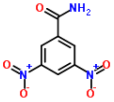
Melting point	**162.00 °C**	**435.15 K**			
CSID	11571	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	183.1216	**H bond donors**	2	**ACD/LogP**	1.74
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.59 g/cm^3
SMILES	O=[N+]([O-])c1cc(cc(N)c1)[N+]([O-])=O				
STD InChIKey	MPBZUKLDHPOCLS-UHFFFAOYAF				

Melting Points

mp °C	source
161.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
163.00	PHYSPROP

3,5-dinitrobenzamide C7H5N3O5[3, 64]

Compound Data



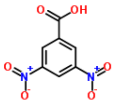
Melting point	**183.00 °C**	**456.15 K**			
CSID	4355	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	211.1317	**H bond donors**	2	**ACD/LogP**	0.55
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.60 g/cm^3
SMILES	O=[N+]([O-])c1cc(cc([N+]([O-])=O)c1)C(=O)N				
STD InChIKey	UUKWKUSGGZNXGA-UHFFFAOYAE				

Melting Points

mp °C	source
182.00	Alfa Aesar
184.00	PHYSPROP

3,5-dinitrobenzoic acid C7H4N2O6[3, 61, 64]

Compound Data



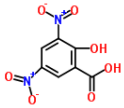
Melting point	**205.67 °C**	**478.82 K**			
CSID	7155	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	212.1165	**H bond donors**	1	**ACD/LogP**	1.69
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.69 g/cm^3
SMILES	O=[N+]([O-])c1cc(cc([N+]([O-])=O)c1)C(=O)O				
STD InChIKey	VYWYYJYRVSBHJQ-UHFFFAOYAQ				

Melting Points

mp °C	source
206.00	Alfa Aesar
206.00	Oxford University MSDS
205.00	PHYSPROP

3,5-dinitrosalicylic acid C7H4N2O7[3, 61, 64]

Compound Data



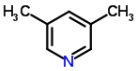
Melting point	**170.50 °C**	**443.65 K**			
CSID	11380	**H bond acceptors**	9	**Rule of 5 violations**	0
Molecular weight	228.12	**H bond donors**	2	**ACD/LogP**	2.71
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.84 g/cm^3
SMILES	c1c(cc(c(c1C(=O)O)O)[N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	LWFUFLREGJMOIZ-UHFFFAOYAQ				

Melting Points

mp °C	source
171.00	Alfa Aesar
170.50	Oxford University MSDS
170.00	PHYSPROP

3,5-lutidine C7H9N[3, 64]

Compound Data



Melting point	**-7.80 °C**	**265.35 K**			
CSID	11077	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.93 g/cm^3
SMILES	n1cc(cc(c1)C)C				
STD InChIKey	HWWYDZCSSYKIAD-UHFFFAOYAB				

Melting Points

mp °C	source
-9.00	Alfa Aesar
-6.60	PHYSPROP

3,5,5-trimethyl-2,4-dioxooxazolidine C6H9NO3[3, 32, 64]

Compound Data

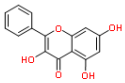
Melting point	**46.33 °C**	**319.48 K**			
CSID	5374	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	143.1406	**H bond donors**	0	**ACD/LogP**	0.31
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.17 g/cm^3
SMILES	O=C1N(C(=O)OC1(C)C)C				
STD InChIKey	IRYJRGCIQBGHIV-UHFFFAOYAZ				

Melting Points

mp °C	source
47.00	Alfa Aesar
46.00	DrugBank
46.00	PHYSPROP

3, 64

3,5,7-trihydroxyflavone C15H10O5



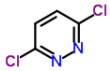
Compound Data

Melting point	**214.75 °C**	**487.90 K**			
CSID	4444935	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	270.2369	**H bond donors**	3	**ACD/LogP**	2.83
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.58 g/cm^3
SMILES	O=C1c3c(O/C(=C1/O)c2ccccc2)cc(O)cc3O				
STD InChIKey	VCCRNZQBSJXYJD-UHFFFAOYAC				

Melting Points

mp °C	source
215.00	Alfa Aesar
214.50	PHYSPROP

3,6-dichloropyridazine C4H2Cl2N2[3, 64]



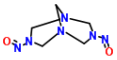
Compound Data

Melting point	**67.75 °C**	**340.90 K**			
CSID	60662	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	148.9781	**H bond donors**	0	**ACD/LogP**	0.90
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	Clc1nnc(Cl)cc1				
STD InChIKey	GUSWJGOYDXFJSI-UHFFFAOYAK				

Melting Points

mp °C	source
68.00	Alfa Aesar
67.50	PHYSPROP

3,7-dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane C5H10N6O2[61, 64]



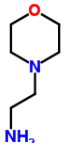
Compound Data

Melting point	**205.75 °C**	**478.90 K**			
CSID	7268	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	186.1719	**H bond donors**	0	**ACD/LogP**	0.05
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.80 g/cm^3
SMILES	O=NN2CN1CN(CN(N=O)C1)C2				
STD InChIKey	MWRWFPQBGSZWNV-UHFFFAOYAW				

Melting Points

mp °C	source
207.00	Oxford University MSDS
204.50	PHYSPROP

4-(2-aminoethyl)morpholine C6H14N2O[3, 64]



Compound Data

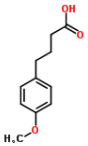
Melting point	**24.80 °C**	**297.95 K**			
CSID	361265	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	130.1882	**H bond donors**	2	**ACD/LogP**	-1.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.00 g/cm^3
SMILES	O1CCN(CCN)CC1				
STD InChIKey	RWIVICVCHVMHMU-UHFFFAOYAF				

Melting Points

mp °C	source
24.00	Alfa Aesar
25.60	PHYSPROP

4-(4-methoxyphenyl)butanoic acid C11H14O3[48, 64]

Compound Data



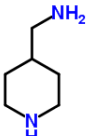
Melting point	**58.25 °C**	**331.40 K**			
CSID	70652	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	194.2271	**H bond donors**	1	**ACD/LogP**	2.33
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.12 g/cm^3
SMILES	O=C(O)CCCc1ccc(OC)cc1				
STD InChIKey	LZHMNCJMXQKSBY-UHFFFAOYAO				

Melting Points

mp °C	source
59.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
57.50	PHYSPROP

4-(aminomethyl)piperidine C6H14N2[3, 64]

Compound Data



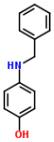
Melting point	**24.50 °C**	**297.65 K**			
CSID	21997	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.1888	**H bond donors**	3	**ACD/LogP**	-0.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.90 g/cm^3
SMILES	NCC1CCNCC1				
STD InChIKey	LTEKQAPRXFBRNN-UHFFFAOYAB				

Melting Points

mp °C	source
24.00	Alfa Aesar
25.00	PHYSPROP

4-(benzylamino)phenol C13H13NO[3, 64]

Compound Data



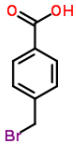
Melting point	**86.00 °C**	**359.15 K**			
CSID	7355	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	199.2484	**H bond donors**	2	**ACD/LogP**	2.38
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.19 g/cm^3
SMILES	Oc2ccc(NCc1ccccc1)cc2				
STD InChIKey	SRYYOKKLTBRLHT-UHFFFAOYAD				

Melting Points

mp °C	source
84.00	Alfa Aesar
88.00	PHYSPROP

4-(bromomethyl)benzoic acid C8H7BrO2[3, 64]

Compound Data



Melting point	**227.50 °C**	**500.65 K**			
CSID	21185	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	215.044	**H bond donors**	1	**ACD/LogP**	2.60
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.64 g/cm^3
SMILES	BrCc1ccc(C(=O)O)cc1				
STD InChIKey	CQQSQBRPAJSTFB-UHFFFAOYAU				

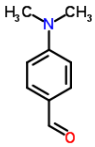
Melting Points

mp °C	source
225.00	Alfa Aesar
230.00	PHYSPROP

4-(dimethylamino)benzaldehyde C9H11NO[2, 3, 35, 48, 61, 64]

Compound Data

Melting point	**74.50 °C**	**347.65 K**			
CSID	7199	**H bond acceptors**	2	**Rule of 5 violations**	0



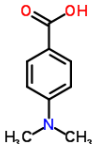
Molecular weight	149.1897	**H bond donors**	0	**ACD/LogP**	1.81
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.07 g/cm^3
SMILES	O=Cc1ccc(N(C)C)cc1				
STD InChIKey	BGNGWHSBYQYVRX-UHFFFAOYAG				

Melting Points

mp °C	source
75.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
74.00	Alfa Aesar
74.50	EPISuite-ChemSpider
75.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
74.00	Oxford University MSDS
74.50	PHYSPROP

4-(dimethylamino)benzoic acid C9H11NO2[61, 64]

Compound Data



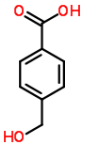
Melting point	**242.75 °C**	**515.90 K**			
CSID	11595	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	165.1891	**H bond donors**	1	**ACD/LogP**	2.31
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	O=C(O)c1ccc(N(C)C)cc1				
STD InChIKey	YDIYEOMDOWUDTJ-UHFFFAOYAK				

Melting Points

mp °C	source
243.00	Oxford University MSDS
242.50	PHYSPROP

4-(hydroxymethyl)benzoic acid C8H8O3[3, 7]

Compound Data



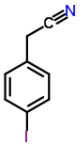
Melting point	**181.50 °C**	**454.65 K**			
CSID	68837	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	0.71
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.31 g/cm^3
SMILES	O=C(O)c1ccc(cc1)CO				
STD InChIKey	WWYFPDXEIFBNKE-UHFFFAOYAK				

Melting Points

mp °C	source
181.00	Alfa Aesar
182.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-(iodophenyl)acetonitrile C8H6IN[3, 7]

Compound Data

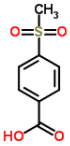


Melting point	**50.50 °C**	**323.65 K**			
CSID	126037	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	243.0444	**H bond donors**	0	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.76 g/cm^3
SMILES	Ic1ccc(cc1)CC#N				
STD InChIKey	PNXWQTYSBFGIFD-UHFFFAOYAN				

Melting Points

mp °C	source
53.00	Alfa Aesar
48.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-(methylsulfonyl)benzoic acid C8H8O4S[3, 64]



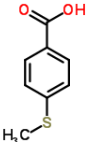
Compound Data

Melting point	**271.25 °C**	**544.40 K**			
CSID	70071	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	200.2117	**H bond donors**	1	**ACD/LogP**	0.67
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	O=S(=O)(c1ccc(C(=O)O)cc1)C				
STD InChIKey	AJBWNNKDUMXZLM-UHFFFAOYAZ				

Melting Points

mp °C	source
273.00	Alfa Aesar
269.50	PHYSPROP

4-(methylthio)benzoic acid C8H8O2S[3, 64]



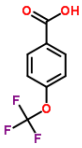
Compound Data

Melting point	**194.75 °C**	**467.90 K**			
CSID	75095	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	168.2129	**H bond donors**	1	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	O=C(O)c1ccc(SC)cc1				
STD InChIKey	KWHCPERWLHBLOT-UHFFFAOYAJ				

Melting Points

mp °C	source
195.00	Alfa Aesar
194.50	PHYSPROP

4-(trifluoromethoxy)benzoic acid C8H5F3O3[3, 64]



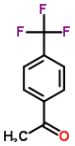
Compound Data

Melting point	**152.50 °C**	**425.65 K**			
CSID	60933	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	206.1187	**H bond donors**	1	**ACD/LogP**	3.00
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.45 g/cm^3
SMILES	FC(F)(F)Oc1ccc(cc1)C(=O)O				
STD InChIKey	RATSANVPHHXDCT-UHFFFAOYAL				

Melting Points

mp °C	source
153.00	Alfa Aesar
152.00	PHYSPROP

4-(trifluoromethyl)acetophenone C9H7F3O[3, 64]



Compound Data

Melting point	**31.50 °C**	**304.65 K**			
CSID	62931	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	188.1465	**H bond donors**	0	**ACD/LogP**	2.60
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	CC(=O)c1ccc(cc1)C(F)(F)F				
STD InChIKey	HHAISVSEJFEWBZ-UHFFFAOYAE				

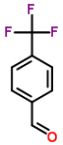
Melting Points

mp °C	source
32.00	Alfa Aesar
31.00	PHYSPROP

4-(trifluoromethyl)benzaldehyde C8H5F3O[3, 3]

Compound Data

Melting point	**1.75 °C**	**274.90 K**



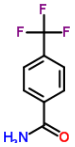
CSID	61311	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	174.1199	**H bond donors**	0	**ACD/LogP**	2.61
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	FC(F)(F)c1ccc(C=O)cc1				
STD InChIKey	BEOBZEOPTQQELP-UHFFFAOYAG				

Melting Points

mp °C	source
1.50	Alfa Aesar
2.00	Alfa Aesar

4-(trifluoromethyl)benzamide C8H6F3NO[3, 64]

Compound Data



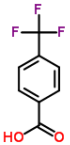
Melting point	**184.50 °C**	**457.65 K**			
CSID	67257	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	189.1345	**H bond donors**	2	**ACD/LogP**	1.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	FC(F)(F)c1ccc(C(=O)N)cc1				
STD InChIKey	WEJHBEDHLLBJFW-UHFFFAOYAB				

Melting Points

mp °C	source
184.00	Alfa Aesar
185.00	PHYSPROP

4-(trifluoromethyl)benzoic acid C8H5F3O2[3, 64]

Compound Data



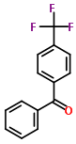
Melting point	**220.25 °C**	**493.40 K**			
CSID	9572	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	190.1193	**H bond donors**	1	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	FC(F)(F)c1ccc(C(=O)O)cc1				
STD InChIKey	SWKPKONEIZGROQ-UHFFFAOYAJ				

Melting Points

mp °C	source
221.00	Alfa Aesar
219.50	PHYSPROP

4-(trifluoromethyl)benzophenone C14H9F3O[3, 48, 64]

Compound Data



Melting point	**116.33 °C**	**389.48 K**			
CSID	62966	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	250.2159	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	FC(F)(F)c2ccc(C(=O)c1ccccc1)cc2				
STD InChIKey	OHTYZZYAMUVKQS-UHFFFAOYAY				

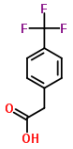
Melting Points

mp °C	source
118.00	Alfa Aesar
116.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
115.00	PHYSPROP

4-(trifluoromethyl)phenylacetic acid C9H7F3O2[3, 64]

Compound Data

Melting point	**82.00 °C**	**355.15 K**



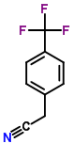
CSID	105768	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	204.1459	**H bond donors**	1	**ACD/LogP**	2.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.36 g/cm^3
SMILES	FC(F)(F)c1ccc(cc1)CC(=O)O				
STD InChIKey	HNORVZDAANCHAY-UHFFFAOYAZ				

Melting Points

mp °C	source
80.00	Alfa Aesar
84.00	PHYSPROP

4-(trifluoromethyl)phenylacetonitrile C9H6F3N[3, 47, 64]

Compound Data



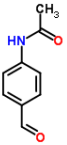
Melting point	**47.17 °C**	**320.32 K**			
CSID	67895	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	185.1458	**H bond donors**	0	**ACD/LogP**	2.02
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	FC(F)(F)c1ccc(cc1)CC#N				
STD InChIKey	QNKOCFJZJWOXDE-UHFFFAOYAE				

Melting Points

mp °C	source
45.00	Alfa Aesar
48.50	IUCr
48.00	PHYSPROP

4-acetamidobenzaldehyde C9H9NO2[3, 7, 64]

Compound Data



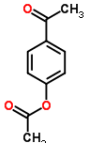
Melting point	**157.67 °C**	**430.82 K**			
CSID	66572	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	163.1733	**H bond donors**	1	**ACD/LogP**	1.25
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.22 g/cm^3
SMILES	O=C(Nc1ccc(cc1)C=O)C				
STD InChIKey	SKLUWKYNZNXSLX-UHFFFAOYAQ				

Melting Points

mp °C	source
156.00	Alfa Aesar
160.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
157.00	PHYSPROP

4-acetoxyacetophenone C10H10O3[3, 7]

Compound Data



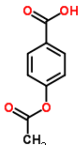
Melting point	**53.50 °C**	**326.65 K**			
CSID	74935	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	178.1846	**H bond donors**	0	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.12 g/cm^3
SMILES	O=C(Oc1ccc(cc1)C(=O)C)C				
STD InChIKey	SMIOEQSLJNNKQF-UHFFFAOYAC				

Melting Points

mp °C	source
53.00	Alfa Aesar
54.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-acetoxybenzoic acid C9H8O4[2, 3, 64]

Compound Data



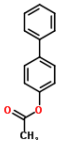
Melting point	**193.50 °C**	**466.65 K**			
CSID	15983	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	180.1574	**H bond donors**	1	**ACD/LogP**	1.48
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.29 g/cm^3
SMILES	O=C(Oc1ccc(cc1)C(=O)O)C				
STD InChIKey	GDBUZIKSJGRBJP-UHFFFAOYAV				

Melting Points

mp °C	source
194.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
194.00	Alfa Aesar
192.50	PHYSPROP

4-acetoxybiphenyl C14H12O2[3, 7, 64]

Compound Data



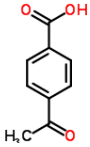
Melting point	**88.33 °C**	**361.48 K**			
CSID	306959	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	0	**ACD/LogP**	3.56
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(Oc1ccc(cc1)c2ccccc2)C				
STD InChIKey	MISFQCBPASYYGV-UHFFFAOYAB				

Melting Points

mp °C	source
88.00	Alfa Aesar
88.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
89.00	PHYSPROP

4-acetylbenzoic acid C9H8O3[2, 3, 64]

Compound Data



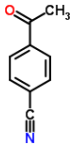
Melting point	**209.00 °C**	**482.15 K**			
CSID	10986	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	164.158	**H bond donors**	1	**ACD/LogP**	1.61
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C(O)c1ccc(C(=O)C)cc1				
STD InChIKey	QBHDSQZASIBAAI-UHFFFAOYAI				

Melting Points

mp °C	source
209.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
210.00	Alfa Aesar
208.00	PHYSPROP

4-acetylbenzonitrile C9H7NO[2, 3, 7, 64]

Compound Data

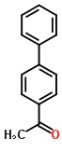


Melting point	**57.88 °C**	**331.02 K**			
CSID	66663	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	145.158	**H bond donors**	0	**ACD/LogP**	1.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	N#Cc1ccc(C(=O)C)cc1				
STD InChIKey	NLPHXWGWBKZSJC-UHFFFAOYAB				

Melting Points

mp °C	source
58.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
57.00	Alfa Aesar
59.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
57.50	PHYSPROP

4-acetylbiphenyl C14H12O[3, 7, 64]



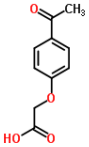
Compound Data

Melting point	**121.00 °C**	**394.15 K**			
CSID	6846	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.2445	**H bond donors**	0	**ACD/LogP**	3.51
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	O=C(c2ccc(c1ccccc1)cc2)C				
STD InChIKey	QCZZSANNLWPGEA-UHFFFAOYAF				

Melting Points

mp °C	source
120.00	Alfa Aesar
122.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
121.00	PHYSPROP

4-acetylphenoxyacetic acid C10H10O4[3, 64]



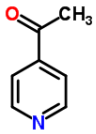
Compound Data

Melting point	**174.50 °C**	**447.65 K**			
CSID	67230	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	1	**ACD/LogP**	0.95
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.24 g/cm^3
SMILES	O=C(c1ccc(OCC(=O)O)cc1)C				
STD InChIKey	KMXZEXUYXUMHEQ-UHFFFAOYAE				

Melting Points

mp °C	source
173.00	Alfa Aesar
176.00	PHYSPROP

4-acetylpyridine C7H7NO[3, 64]



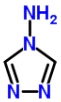
Compound Data

Melting point	**15.50 °C**	**288.65 K**			
CSID	13644	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	121.1366	**H bond donors**	0	**ACD/LogP**	0.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.06 g/cm^3
SMILES	O=C(c1ccncc1)C				
STD InChIKey	WMQUKDQWMMOHSA-UHFFFAOYAX				

Melting Points

mp °C	source
15.00	Alfa Aesar
16.00	PHYSPROP

4-amino-1,2,4-triazole C2H4N4[3, 64]



Compound Data

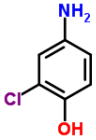
Melting point	**84.25 °C**	**357.40 K**			
CSID	10951	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	84.08	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.60 g/cm^3
SMILES	c1nncn1N				
STD InChIKey	FMCUPJKTGNBGEC-UHFFFAOYAB				

Melting Points

mp °C	source
86.00	Alfa Aesar
82.50	PHYSPROP

4-amino-2-chlorophenol C6H6ClNO[3, 61]

Compound Data



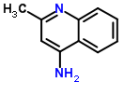
Melting point	**151.75 °C**	**424.90 K**			
CSID	69983	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	143.5709	**H bond donors**	3	**ACD/LogP**	0.55
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Clc1cc(N)ccc1O				
STD InChIKey	ZYZQSCWSPFLAFM-UHFFFAOYAH				

Melting Points

mp °C	source
152.00	Alfa Aesar
151.50	Oxford University MSDS

4-amino-2-methylquinoline C10H10N2[3, 64]

Compound Data



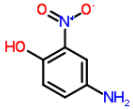
Melting point	**166.50 °C**	**439.65 K**			
CSID	73183	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.1998	**H bond donors**	2	**ACD/LogP**	2.09
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	n1c(cc(c2ccccc12)N)C				
STD InChIKey	COCFIBRMFPWUDW-UHFFFAOYAZ				

Melting Points

mp °C	source
164.00	Alfa Aesar
169.00	PHYSPROP

4-amino-2-nitrophenol C6H6N2O3[3, 64]

Compound Data



Melting point	**127.50 °C**	**400.65 K**			
CSID	2661194	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	154.1234	**H bond donors**	3	**ACD/LogP**	0.64
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.51 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1O)N				
STD InChIKey	WHODQVWERNSQEO-UHFFFAOYAM				

Melting Points

mp °C	source
129.00	Alfa Aesar
126.00	PHYSPROP

4-amino-2,6-dichlorophenol C6H5Cl2NO[3, 61, 64]

Compound Data

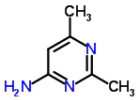
Melting point	**167.83 °C**	**440.98 K**			
CSID	72291	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	178.016	**H bond donors**	3	**ACD/LogP**	1.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.56 g/cm^3
SMILES	Clc1cc(cc(Cl)c1O)N				
STD InChIKey	KGEXISHTCZHGFT-UHFFFAOYAM				

Melting Points

mp °C	source
167.00	Alfa Aesar
168.50	Oxford University MSDS
168.00	PHYSPROP

4-amino-2,6-dimethylpyrimidine C6H9N3[3, 64]

Compound Data



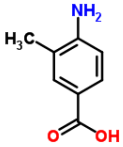
Melting point	**184.00 °C**	**457.15 K**			
CSID	61354	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	123.1558	**H bond donors**	2	**ACD/LogP**	0.39
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	n1c(cc(nc1C)N)C				
STD InChIKey	BJJDXAFKCKSLTE-UHFFFAOYAV				

Melting Points

mp °C	source
185.00	Alfa Aesar
183.00	PHYSPROP

4-amino-3-methylbenzoic acid C8H9NO2[3, 64]

Compound Data



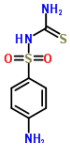
Melting point	**169.75 °C**	**442.90 K**			
CSID	68122	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	3	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	O=C(O)c1ccc(N)c(c1)C				
STD InChIKey	NHFKECPTBZZFBC-UHFFFAOYAZ				

Melting Points

mp °C	source
170.00	Alfa Aesar
169.50	PHYSPROP

4-amino-N-carbamothioylbenzenesulfonamide C7H9N3O2S2[64, 64]

Compound Data



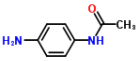
Melting point	**180.50 °C**	**453.65 K**			
CSID	2272143	**H bond acceptors**	5	**Rule of 5 violations**	1
Molecular weight	231.2953	**H bond donors**	5	**ACD/LogP**	-0.48
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.53 g/cm^3
SMILES	O=S(=O)(c1ccc(N)cc1)NC(=S)N				
STD InChIKey	UEMLYRZWLVXWRU-UHFFFAOYAW				

Melting Points

mp °C	source
182.00	PHYSPROP
179.00	PHYSPROP

4-aminoacetanilide C8H10N2O[3, 64]

Compound Data



Melting point	**164.75 °C**	**437.90 K**			
CSID	10297844	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1778	**H bond donors**	3	**ACD/LogP**	0.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	Nc1ccc(NC(C)=O)cc1				
STD InChIKey	CHMBIJAOCISYEW-UHFFFAOYAK				

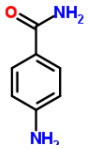
Melting Points

mp °C	source
163.00	Alfa Aesar
166.50	PHYSPROP

4-aminobenzamide C7H8N2O[2, 3, 64]

Compound Data

Melting point	**182.33 °C**	**455.48 K**			
CSID	68568	**H bond acceptors**	3	**Rule of 5 violations**	0



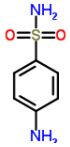
Molecular weight	136.1512	**H bond donors**	4	**ACD/LogP**	0.09
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C(c1ccc(N)cc1)N				
STD InChIKey	QIKYZXDTTPVVAC-UHFFFAOYAB				

Melting Points

mp °C	source
182.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
183.00	Alfa Aesar
182.00	PHYSPROP

4-aminobenzenesulfonamide C6H8N2O2S[3, 32, 44, 61, 64]

Compound Data



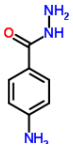
Melting point	**165.50 °C**	**438.65 K**			
CSID	5142	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.2049	**H bond donors**	4	**ACD/LogP**	-0.72
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.43 g/cm^3
SMILES	O=S(=O)(c1ccc(N)cc1)N				
STD InChIKey	FDDDEECHVMSUSB-UHFFFAOYAI				

Melting Points

mp °C	source
166.00	Alfa Aesar
165.50	DrugBank
165.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
165.00	Oxford University MSDS
165.50	PHYSPROP

4-aminobenzhydrazide C7H9N3O[3, 64]

Compound Data



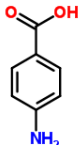
Melting point	**227.00 °C**	**500.15 K**			
CSID	20160	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	151.1659	**H bond donors**	5	**ACD/LogP**	-0.75
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	O=C(c1ccc(N)cc1)NN				
STD InChIKey	WPBZMCGPFHZRHJ-UHFFFAOYAL				

Melting Points

mp °C	source
228.00	Alfa Aesar
226.00	PHYSPROP

4-aminobenzoic acid C7H7NO2[2, 3, 32, 35, 44, 61, 64, 70, 70]

Compound Data



Melting point	**188.53 °C**	**461.68 K**			
CSID	953	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	3	**ACD/LogP**	0.83
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=C(O)c1ccc(N)cc1				
STD InChIKey	ALYNCZNDIQEVRV-UHFFFAOYAH				

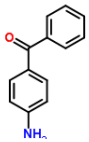
Melting Points

mp °C	source
189.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
188.00	Alfa Aesar
188.50	DrugBank
188.50	EPISuite-ChemSpider

187.80	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
188.50	Oxford University MSDS
188.50	PHYSPROP
189.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
189.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

4-aminobenzophenone C13H11NO[3, 64]

Compound Data



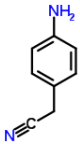
Melting point	**122.75 °C**	**395.90 K**			
CSID	13707	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	197.2325	**H bond donors**	2	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	O=C(c1ccc(N)cc1)c2ccccc2				
STD InChIKey	RBKHNGHPZZZJCI-UHFFFAOYAH				

Melting Points

mp °C	source
123.00	Alfa Aesar
122.50	PHYSPROP

4-aminobenzyl cyanide C8H8N2[2, 2, 3, 64]

Compound Data



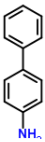
Melting point	**44.75 °C**	**317.90 K**			
CSID	69446	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	132.1625	**H bond donors**	2	**ACD/LogP**	0.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.12 g/cm^3
SMILES	N#CCc1ccc(N)cc1				
STD InChIKey	YCWRFIYBUQBHJI-UHFFFAOYAP				

Melting Points

mp °C	source
44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
45.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
44.00	Alfa Aesar
46.00	PHYSPROP

4-aminobiphenyl C12H11N[7, 61, 64]

Compound Data



Melting point	**53.50 °C**	**326.65 K**			
CSID	6835	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	169.2224	**H bond donors**	2	**ACD/LogP**	2.77
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.08 g/cm^3
SMILES	c2c(c1ccc(N)cc1)cccc2				
STD InChIKey	DMVOXQPQNTYEKQ-UHFFFAOYAX				

Melting Points

mp °C	source
54.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
53.00	Oxford University MSDS
53.50	PHYSPROP

4-aminophenol C6H7NO[2, 3, 61, 64]

Compound Data

Melting point	**188.38 °C**	**461.52 K**			
CSID	392	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	3	**ACD/LogP**	0.01
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3

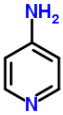
SMILES	c1cc(ccc1N)O
STD InChIKey	PLIKAWJENQZMHA-UHFFFAOYAD

Melting Points

mp °C	source
189.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
188.00	Alfa Aesar
189.00	Oxford University MSDS
187.50	PHYSPROP

4-aminopyridine C5H6N2[3, 64]

Compound Data



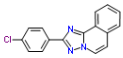
Melting point	**158.75 °C**	**431.90 K**			
CSID	1664	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.1145	**H bond donors**	2	**ACD/LogP**	0.26
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	n1ccc(N)cc1				
STD InChIKey	NUKYPUAOHBNCPY-UHFFFAOYAH				

Melting Points

mp °C	source
159.00	Alfa Aesar
158.50	PHYSPROP

4-aminopyrimidine C16H10ClN3[9, 48, 64]

Compound Data



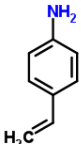
Melting point	**238.33 °C**	**511.48 K**			
CSID	62098	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	279.7237	**H bond donors**	0	**ACD/LogP**	5.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	Clc4ccc(c1nc2c3c(ccn2n1)cccc3)cc4				
STD InChIKey	DGWUVKLBXCWNTA-UHFFFAOYAQ				

Melting Points

mp °C	source
238.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
238.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
239.00	PHYSPROP

4-aminostyrene C8H9N[3, 7, 64]

Compound Data

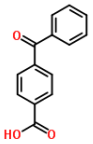


Melting point	**24.50 °C**	**297.65 K**			
CSID	66344	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	119.1638	**H bond donors**	2	**ACD/LogP**	1.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.01 g/cm^3
SMILES	C=C\c1ccc(N)cc1				
STD InChIKey	LBSXSAXOLABXMF-UHFFFAOYAN				

Melting Points

mp °C	source
24.00	Alfa Aesar
26.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
23.50	PHYSPROP

4-benzoylbenzoic acid C14H10O3[3, 61, 64]



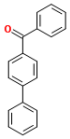
Compound Data

Melting point	**198.67 °C**	**471.82 K**			
CSID	62362	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.2274	**H bond donors**	1	**ACD/LogP**	3.29
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.26 g/cm^3
SMILES	O=C(O)c2ccc(C(=O)c1ccccc1)cc2				
STD InChIKey	IFQUPKAISSPFTE-UHFFFAOYAO				

Melting Points

mp °C	source
199.00	Alfa Aesar
198.00	Oxford University MSDS
199.00	PHYSPROP

4-benzoylbiphenyl C19H14O[3, 64]



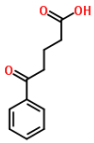
Compound Data

Melting point	**100.50 °C**	**373.65 K**			
CSID	67593	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	258.3139	**H bond donors**	0	**ACD/LogP**	5.37
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=C(c2ccc(c1ccccc1)cc2)c3ccccc3				
STD InChIKey	LYXOWKPVTCPORE-UHFFFAOYAO				

Melting Points

mp °C	source
101.00	Alfa Aesar
100.00	PHYSPROP

4-benzoylbutyric acid C11H12O3[3, 64]



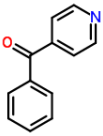
Compound Data

Melting point	**127.12 °C**	**400.27 K**			
CSID	66547	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	192.2112	**H bond donors**	1	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.16 g/cm^3
SMILES	O=C(c1ccccc1)CCCC(=O)O				
STD InChIKey	SHKWSBAVRQZYLE-UHFFFAOYAT				

Melting Points

mp °C	source
127.00	Alfa Aesar
127.25	PHYSPROP

4-benzoylpyridine C12H9NO[3, 64]



Compound Data

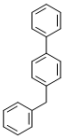
Melting point	**71.00 °C**	**344.15 K**			
CSID	24905	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	183.206	**H bond donors**	0	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(c1ccccc1)c2ccncc2				
STD InChIKey	SKFLCXNDKRUHTA-UHFFFAOYAL				

Melting Points

mp °C	source
70.00	Alfa Aesar
72.00	PHYSPROP

4-benzylbiphenyl C19H16[3, 64]

Compound Data



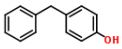
Melting point	**85.50 °C**	**358.65 K**			
CSID	62389	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	244.3303	**H bond donors**	0	**ACD/LogP**	5.96
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.04 g/cm^3
SMILES	c1c(cccc1)Cc2ccc(cc2)c3ccccc3				
STD InChIKey	AGPLQTQFIZBOLI-UHFFFAOYAY				

Melting Points

mp °C	source
86.00	Alfa Aesar
85.00	PHYSPROP

4-benzylphenol C13H12O[3, 64]

Compound Data



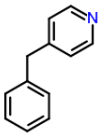
Melting point	**83.50 °C**	**356.65 K**			
CSID	21159439	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.2338	**H bond donors**	1	**ACD/LogP**	3.47
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	Oc2ccc(Cc1ccccc1)cc2				
STD InChIKey	HJSPWKGEPDZNLK-UHFFFAOYAX				

Melting Points

mp °C	source
83.00	Alfa Aesar
84.00	PHYSPROP

4-benzylpyridine C12H11N[3, 64]

Compound Data



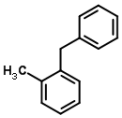
Melting point	**11.20 °C**	**284.35 K**			
CSID	15603	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	169.2224	**H bond donors**	0	**ACD/LogP**	2.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	n1ccc(cc1)Cc2ccccc2				
STD InChIKey	DBOLXXRVIFGDTI-UHFFFAOYAL				

Melting Points

mp °C	source
10.00	Alfa Aesar
12.40	PHYSPROP

4-benzyltoluene C14H14[4, 64]

Compound Data



Melting point	**6.80 °C**	**279.95 K**			
CSID	62938	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.98 g/cm^3
SMILES	c1c(cccc1)Cc2ccccc2C				
STD InChIKey	PQTAUFTUHHRKSS-UHFFFAOYAY				

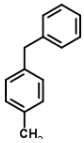
Melting Points

mp °C	source
7.00	American Petroleum Institute. Research Project 44; Selected ...
6.60	PHYSPROP

4-benzyltoluene C14H14[4, 53, 59, 59, 64, 64, 76]

Compound Data

Melting point	**4.86 °C**	**278.01 K**			
CSID	62501	**H bond acceptors**	0	**Rule of 5 violations**	0



Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.98 g/cm^3
SMILES	c1c(cccc1)Cc2ccc(cc2)C				
STD InChIKey	SIYISNUJKMAQBV-UHFFFAOYAZ				

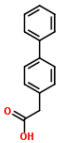
Melting Points

mp °C	source
5.00	American Petroleum Institute. Research Project 44; Selected ...
4.58	NIST Web Book
5.00	UsefulChem EXP266
	Values not used in calculating the average melting point
97.50	Manih RM; Myrboh B. Indian Journal of Chemistry 48B(1) 146-1...[1]
-30.00	NIST Web Book[2]
-30.00	PHYSPROP[3]
125.00	PHYSPROP[4]

1. clearly a liquid at rt http://usefulchem.wikispaces.com/Exp266 JCB
2. freezes at -15C after 16 days http://usefulchem.wikispaces.com/Exp266 JCB
3. freezes at -15C after 16 days http://usefulchem.wikispaces.com/Exp266 JCB
4. clearly a liquid at rt http://usefulchem.wikispaces.com/Exp266 JCB

4-biphenylacetic acid C14H12O2[3, 64]

Compound Data



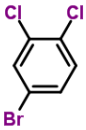
Melting point	**160.75 °C**	**433.90 K**			
CSID	3215	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	1	**ACD/LogP**	3.26
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)Cc1ccc(cc1)c2ccccc2				
STD InChIKey	QRZAKQDHEVVFRX-UHFFFAOYAC				

Melting Points

mp °C	source
161.00	Alfa Aesar
160.50	PHYSPROP

4-bromo-1,2-dichlorobenzene C6H3BrCl2[3, 64]

Compound Data



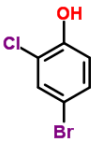
Melting point	**24.50 °C**	**297.65 K**			
CSID	13881395	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	225.898	**H bond donors**	0	**ACD/LogP**	3.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.74 g/cm^3
SMILES	Clc1cc(Br)ccc1Cl				
STD InChIKey	CFPZDVAZISWERM-UHFFFAOYAW				

Melting Points

mp °C	source
24.00	Alfa Aesar
25.00	PHYSPROP

4-bromo-2-chlorophenol C6H4BrClO[3, 64]

Compound Data



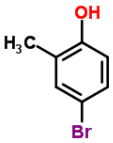
Melting point	**49.75 °C**	**322.90 K**			
CSID	18707	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	207.4524	**H bond donors**	1	**ACD/LogP**	3.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.79 g/cm^3
SMILES	Clc1cc(Br)ccc1O				
STD InChIKey	VIBJPUXLAKVICD-UHFFFAOYAV				

Melting Points

mp °C	source
49.00	Alfa Aesar
50.50	PHYSPROP

4-bromo-2-methylphenol C7H7BrO[3, 64]

Compound Data



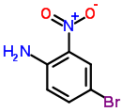
Melting point	**64.35 °C**	**337.50 K**			
CSID	16011	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	187.0339	**H bond donors**	1	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.55 g/cm^3
SMILES	Brc1cc(c(O)cc1)C				
STD InChIKey	IWJGMJHAIUBWKT-UHFFFAOYAK				

Melting Points

mp °C	source
64.00	Alfa Aesar
64.70	PHYSPROP

4-bromo-2-nitroaniline C6H5BrN2O2[3, 64]

Compound Data



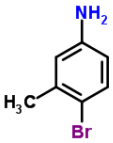
Melting point	**111.75 °C**	**384.90 K**			
CSID	63320	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	217.0201	**H bond donors**	2	**ACD/LogP**	2.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.81 g/cm^3
SMILES	Brc1cc([N+]([O-])=O)c(N)cc1				
STD InChIKey	ZCWBZRBJSPWUPG-UHFFFAOYAV				

Melting Points

mp °C	source
112.00	Alfa Aesar
111.50	PHYSPROP

4-bromo-3-methylaniline C7H8BrN[2, 3, 64]

Compound Data



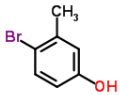
Melting point	**80.33 °C**	**353.48 K**			
CSID	21844	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	186.0491	**H bond donors**	2	**ACD/LogP**	2.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.50 g/cm^3
SMILES	Brc1ccc(N)cc1C				
STD InChIKey	MMEGELSFOYDPQW-UHFFFAOYAJ				

Melting Points

mp °C	source
79.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
81.00	Alfa Aesar
81.00	PHYSPROP

4-bromo-3-methylphenol C7H7BrO[3, 48, 64]

Compound Data



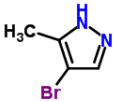
Melting point	**62.17 °C**	**335.32 K**			
CSID	65689	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	187.0339	**H bond donors**	1	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.55 g/cm^3
SMILES	Brc1ccc(O)cc1C				
STD InChIKey	GPOQODYGMUTOQL-UHFFFAOYAN				

Melting Points

mp °C	source
59.00	Alfa Aesar
64.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
63.50	PHYSPROP

4-bromo-3-methylpyrazole C4H5BrN2[3, 64]

Compound Data



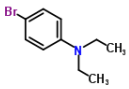
Melting point	**75.75 °C**	**348.90 K**			
CSID	75563	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.9999	**H bond donors**	1	**ACD/LogP**	1.55
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.72 g/cm^3
SMILES	Brc1cnnc1C				
STD InChIKey	IXQPRETWBGVNPJ-UHFFFAOYAW				

Melting Points

mp °C	source
75.00	Alfa Aesar
76.50	PHYSPROP

4-bromo-N,N-diethylaniline C10H14BrN[3, 64]

Compound Data



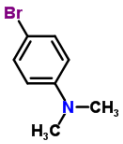
Melting point	**36.00 °C**	**309.15 K**			
CSID	21159579	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	228.1289	**H bond donors**	0	**ACD/LogP**	4.40
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.29 g/cm^3
SMILES	Brc1ccc(cc1)N(CC)CC				
STD InChIKey	NGYMZFJVHHKJQR-UHFFFAOYAE				

Melting Points

mp °C	source
34.00	Alfa Aesar
38.00	PHYSPROP

4-bromo-N,N-dimethylaniline C8H10BrN[2, 3, 64]

Compound Data



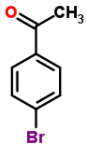
Melting point	**54.67 °C**	**327.82 K**			
CSID	13873600	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	200.0757	**H bond donors**	0	**ACD/LogP**	3.34
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	CN(C)c1ccc(Br)cc1				
STD InChIKey	XYZWMVYYUIMRIZ-UHFFFAOYAU				

Melting Points

mp °C	source
55.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
55.00	PHYSPROP

4-bromoacetophenone C8H7BrO[2, 3, 64]

Compound Data

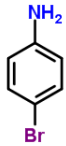


Melting point	**50.83 °C**	**323.98 K**			
CSID	7186	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	199.0446	**H bond donors**	0	**ACD/LogP**	2.43
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.45 g/cm^3
SMILES	CC(=O)c1ccc(cc1)Br				
STD InChIKey	WYECURVXVYPVAT-UHFFFAOYAE				

Melting Points

mp °C	source
51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
51.00	Alfa Aesar
50.50	PHYSPROP

4-bromoaniline C6H6BrN[2, 3, 61, 64]



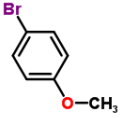
Compound Data

Melting point	**64.10 °C**	**337.25 K**			
CSID	7519	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	172.0225	**H bond donors**	2	**ACD/LogP**	2.05
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.59 g/cm^3
SMILES	Brc1ccc(N)cc1				
STD InChIKey	WDFQBORIUYODSI-UHFFFAOYAG				

Melting Points

mp °C	source
63.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
63.00	Alfa Aesar
64.00	Oxford University MSDS
66.40	PHYSPROP

4-bromoanisole C7H7BrO[2, 3, 64]



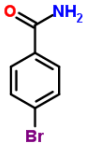
Compound Data

Melting point	**11.50 °C**	**284.65 K**			
CSID	13881571	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	187.0339	**H bond donors**	0	**ACD/LogP**	3.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.44 g/cm^3
SMILES	COc1ccc(cc1)Br				
STD InChIKey	QJPJQTDYNZXKQF-UHFFFAOYAK				

Melting Points

mp °C	source
10.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
11.00	Alfa Aesar
13.50	PHYSPROP

4-bromobenzamide C7H6BrNO[2, 3, 64]



Compound Data

Melting point	**191.50 °C**	**464.65 K**			
CSID	62884	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.0326	**H bond donors**	2	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.61 g/cm^3
SMILES	O=C(c1ccc(Br)cc1)N				
STD InChIKey	ZRWNRAJCPNLYAK-UHFFFAOYAB				

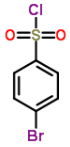
Melting Points

mp °C	source
191.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
192.00	Alfa Aesar
191.50	PHYSPROP

4-bromobenzenesulfonyl chloride C6H4BrClO2S[3, 64]

Compound Data

Melting point	**75.50 °C**	**348.65 K**			
CSID	7118	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	255.5168	**H bond donors**	0	**ACD/LogP**	3.02
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.79 g/cm^3



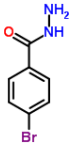
SMILES	O=S(Cl)(=O)c1ccc(Br)cc1
STD InChIKey	KMMHZIBWCXYAAH-UHFFFAOYAQ

Melting Points

mp °C	source
75.00	Alfa Aesar
76.00	PHYSPROP

4-bromobenzhydrazide C7H7BrN2O[3, 64]

Compound Data



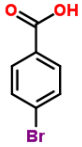
Melting point	**167.00 °C**	**440.15 K**			
CSID	20861	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	215.0473	**H bond donors**	3	**ACD/LogP**	1.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.61 g/cm^3
SMILES	O=C(c1ccc(Br)cc1)NN				
STD InChIKey	UYIMBYKIIMYFPS-UHFFFAOYAQ				

Melting Points

mp °C	source
168.00	Alfa Aesar
166.00	PHYSPROP

4-bromobenzoic acid C7H5BrO2[2, 3, 64, 70]

Compound Data



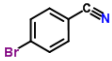
Melting point	**253.88 °C**	**527.02 K**			
CSID	10980	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	201.0174	**H bond donors**	1	**ACD/LogP**	2.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.70 g/cm^3
SMILES	O=C(O)c1ccc(Br)cc1				
STD InChIKey	TUXYZHVUPGXXQG-UHFFFAOYAX				

Melting Points

mp °C	source
253.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
256.00	Alfa Aesar
254.50	PHYSPROP
252.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

4-bromobenzonitrile C7H4BrN[2, 3, 64]

Compound Data

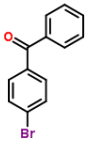


Melting point	**112.67 °C**	**385.82 K**			
CSID	11662	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.0174	**H bond donors**	0	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.61 g/cm^3
SMILES	c1cc(ccc1C#N)Br				
STD InChIKey	HQSCPPCMBMFJJN-UHFFFAOYAP				

Melting Points

mp °C	source
111.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
113.00	Alfa Aesar
114.00	PHYSPROP

4-bromobenzophenone C13H9BrO[2, 3, 64]



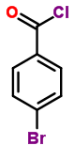
Compound Data

Melting point	**81.83 °C**	**354.98 K**			
CSID	6763	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	261.114	**H bond donors**	0	**ACD/LogP**	4.12
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.42 g/cm^3
SMILES	O=C(c1ccc(Br)cc1)c2ccccc2				
STD InChIKey	KEOLYBMGRQYQTN-UHFFFAOYAW				

Melting Points

mp °C	source
82.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
81.00	Alfa Aesar
82.50	PHYSPROP

4-bromobenzoyl chloride C7H4BrClO[3, 64]



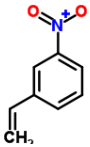
Compound Data

Melting point	**41.00 °C**	**314.15 K**			
CSID	61790	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	219.4631	**H bond donors**	0	**ACD/LogP**	3.15
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.66 g/cm^3
SMILES	O=C(Cl)c1ccc(Br)cc1				
STD InChIKey	DENKGPBHLYFNGK-UHFFFAOYAR				

Melting Points

mp °C	source
40.00	Alfa Aesar
42.00	PHYSPROP

4-bromobenzoyl chloride C8H7NO2[2, 3, 61, 64]



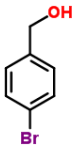
Compound Data

Melting point	**-6.25 °C**	**266.90 K**			
CSID	61789	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	149.1467	**H bond donors**	0	**ACD/LogP**	2.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=[N+]([O-])c1cc(\C=C)ccc1				
STD InChIKey	SYZVQXIUVGKCBJ-UHFFFAOYAN				

Melting Points

mp °C	source
-5.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-5.00	Alfa Aesar
-5.00	Oxford University MSDS
-10.00	PHYSPROP

4-bromobenzyl alcohol C7H7BrO[2, 3]



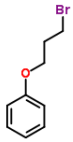
Compound Data

Melting point	**77.00 °C**	**350.15 K**			
CSID	63307	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	187.0339	**H bond donors**	1	**ACD/LogP**	1.81
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.56 g/cm^3
SMILES	Brc1ccc(cc1)CO				
STD InChIKey	VEDDBHYQWFOITD-UHFFFAOYAD				

Melting Points

mp °C	source
76.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
78.00	Alfa Aesar

4-bromobenzyl bromide C9H11BrO[3, 64]



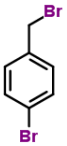
Compound Data

Melting point	**10.35 °C**	**283.50 K**			
CSID	61797	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	215.087	**H bond donors**	0	**ACD/LogP**	3.29
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.35 g/cm^3
SMILES	BrCCCOc1ccccc1				
STD InChIKey	NIDWUZTTXGJFNN-UHFFFAOYAV				

Melting Points

mp °C	source
10.00	Alfa Aesar
10.70	PHYSPROP

4-bromobenzyl bromide C7H6Br2[3, 64]



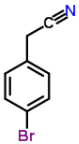
Compound Data

Melting point	**62.50 °C**	**335.65 K**			
CSID	61802	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	249.9305	**H bond donors**	0	**ACD/LogP**	3.69
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.85 g/cm^3
SMILES	BrCc1ccc(Br)cc1				
STD InChIKey	YLRBJYMANQKEAW-UHFFFAOYAE				

Melting Points

mp °C	source
62.00	Alfa Aesar
63.00	PHYSPROP

4-bromobenzyl cyanide C8H6BrN[2, 3, 64]



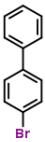
Compound Data

Melting point	**47.67 °C**	**320.82 K**			
CSID	25968	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.0439	**H bond donors**	0	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.49 g/cm^3
SMILES	Brc1ccc(cc1)CC#N				
STD InChIKey	MFHFWRBXPQDZSA-UHFFFAOYAA				

Melting Points

mp °C	source
48.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
47.00	Alfa Aesar
48.00	PHYSPROP

4-bromobiphenyl C12H9Br[3, 64]



Compound Data

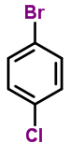
Melting point	**90.75 °C**	**363.90 K**			
CSID	6834	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	233.1039	**H bond donors**	0	**ACD/LogP**	4.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	Brc2ccc(c1ccccc1)cc2				
STD InChIKey	PKJBWOWQJHHAHG-UHFFFAOYAK				

Melting Points

mp °C	source
90.00	Alfa Aesar
91.50	PHYSPROP

4-bromochlorobenzene C6H4BrCl[2, 3, 64]

Compound Data



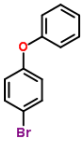
Melting point	**66.67 °C**	**339.82 K**			
CSID	7518	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	191.453	**H bond donors**	0	**ACD/LogP**	3.52
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.63 g/cm^3
SMILES	Clc1ccc(Br)cc1				
STD InChIKey	NHDODQWIKUYWMW-UHFFFAOYAV				

Melting Points

mp °C	source
67.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
65.00	Alfa Aesar
68.00	PHYSPROP

4-bromodiphenyl ether C12H9BrO[3, 64]

Compound Data



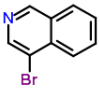
Melting point	**18.36 °C**	**291.51 K**			
CSID	7284	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	249.1033	**H bond donors**	0	**ACD/LogP**	5.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Brc2ccc(Oc1ccccc1)cc2				
STD InChIKey	JDUYPUMQALQRCN-UHFFFAOYAP				

Melting Points

mp °C	source
18.00	Alfa Aesar
18.72	PHYSPROP

4-bromoisoquinoline C9H6BrN[3, 64]

Compound Data



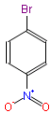
Melting point	**41.25 °C**	**314.40 K**			
CSID	66385	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	208.0546	**H bond donors**	0	**ACD/LogP**	2.98
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.56 g/cm^3
SMILES	Brc2c1c(cccc1)cnc2				
STD InChIKey	SCRBSGZBTHKAHU-UHFFFAOYAW				

Melting Points

mp °C	source
41.00	Alfa Aesar
41.50	PHYSPROP

4-bromonitrobenzene C6H4BrNO2[2, 3, 64]

Compound Data



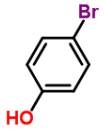
Melting point	**126.33 °C**	**399.48 K**			
CSID	21171513	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	202.0055	**H bond donors**	0	**ACD/LogP**	2.55
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.72 g/cm^3
SMILES	O=[N+]([O-])c1ccc(Br)cc1				
STD InChIKey	ZDFBKZUDCQQKAC-UHFFFAOYAB				

Melting Points

mp °C	source
126.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
126.00	Alfa Aesar
127.00	PHYSPROP

4-bromophenol C6H5BrO[2, 3, 64, 72]

Compound Data



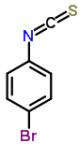
Melting point	**64.72 °C**	**337.88 K**			
CSID	13842573	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	173.0073	**H bond donors**	1	**ACD/LogP**	2.49
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.66 g/cm^3
SMILES	Oc1ccc(Br)cc1				
STD InChIKey	GZFGOTFRPZRKDS-UHFFFAOYAE				

Melting Points

mp °C	source
66.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
64.00	Alfa Aesar
66.40	PHYSPROP
62.50	Sigma-Aldrich

4-bromophenyl isothiocyanate C7H4BrNS[3, 64]

Compound Data



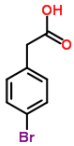
Melting point	**59.25 °C**	**332.40 K**			
CSID	15317	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	214.0824	**H bond donors**	0	**ACD/LogP**	4.03
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.50 g/cm^3
SMILES	Brc1ccc(\N=C=S)cc1				
STD InChIKey	XQACWEBGSZBLRG-UHFFFAOYAV				

Melting Points

mp °C	source
58.00	Alfa Aesar
60.50	PHYSPROP

4-bromophenylacetic acid C8H7BrO2[3, 35, 64]

Compound Data



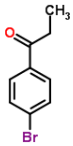
Melting point	**116.33 °C**	**389.48 K**			
CSID	67229	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	215.044	**H bond donors**	1	**ACD/LogP**	2.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.62 g/cm^3
SMILES	Brc1ccc(cc1)CC(=O)O				
STD InChIKey	QOWSWEBLNVACCL-UHFFFAOYAS				

Melting Points

mp °C	source
117.00	Alfa Aesar
116.00	EPISuite-ChemSpider
116.00	PHYSPROP

4-bromopropiophenone C9H9BrO[3, 64]

Compound Data

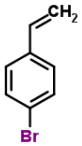


Melting point	**47.00 °C**	**320.15 K**			
CSID	59691	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	213.0712	**H bond donors**	0	**ACD/LogP**	2.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	O=C(c1ccc(Br)cc1)CC				
STD InChIKey	UOMOSYFPKGQIKI-UHFFFAOYAL				

Melting Points

mp °C	source
46.00	Alfa Aesar
48.00	PHYSPROP

4-bromostyrene C8H7Br[3, 64]



Compound Data

Melting point	**6.35 °C**	**279.50 K**			
CSID	15431	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	183.0452	**H bond donors**	0	**ACD/LogP**	3.59
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.39 g/cm^3
SMILES	Brc1ccc(\C=C)cc1				
STD InChIKey	WGGLDBIZIQMEGH-UHFFFAOYAY				

Melting Points

mp °C	source
5.00	Alfa Aesar
7.70	PHYSPROP

4-bromothiophenol C6H5BrS[3, 64]

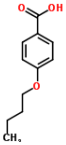
Compound Data

Melting point	**74.00 °C**	**347.15 K**			
CSID	59439	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	189.0729	**H bond donors**	0	**ACD/LogP**	3.53
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.60 g/cm^3
SMILES	Brc1ccc(S)cc1				
STD InChIKey	FTBCOQFMQSTCQQ-UHFFFAOYAM				

Melting Points

mp °C	source
75.00	Alfa Aesar
73.00	PHYSPROP

4-butoxybenzoic acid C11H14O3[2, 64]



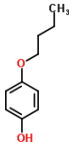
Compound Data

Melting point	**147.75 °C**	**420.90 K**			
CSID	65785	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	194.2271	**H bond donors**	1	**ACD/LogP**	3.55
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.11 g/cm^3
SMILES	O=C(O)c1ccc(OCCCC)cc1				
STD InChIKey	LAUFPZPAKULAGB-UHFFFAOYAE				

Melting Points

mp °C	source
147.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
148.50	PHYSPROP

4-butoxyphenol C10H14O2[2, 64]



Compound Data

Melting point	**65.25 °C**	**338.40 K**			
CSID	28973	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	166.217	**H bond donors**	1	**ACD/LogP**	2.90
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.03 g/cm^3
SMILES	O(c1ccc(O)cc1)CCCC				
STD InChIKey	MBGGFXOXUIDRJD-UHFFFAOYAH				

Melting Points

mp °C	source
65.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
65.50	PHYSPROP

4-chlor-2-methoxyanilin C7H8ClNO[2, 64]

Compound Data

Melting point	**51.50 °C**	**324.65 K**

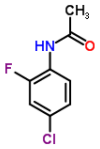
CSID	21159424	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	157.5975	**H bond donors**	2	**ACD/LogP**	2.14
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	Nc1ccc(Cl)cc1OC				
STD InChIKey	WOXLPNAOCCIZGP-UHFFFAOYAL				

Melting Points

mp °C	source
51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
52.00	PHYSPROP

4-chloro-2-fluoroacetanilide C8H7ClFNO[3, 22, 23, 64]

Compound Data



Melting point	**156.00 °C**	**429.15 K**			
CSID	745600	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	187.5987	**H bond donors**	1	**ACD/LogP**	1.43
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	Clc1cc(F)c(NC(=O)C)cc1				
STD InChIKey	GVRKNSAEOVXHOS-UHFFFAOYAV				

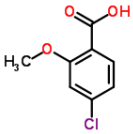
Melting Points

mp °C	source
156.00	Alfa Aesar
155.00	ChemKoo
157.00	ChemNet
	Values not used in calculating the average melting point
48.50	PHYSPROP[1]

1. clearly out of range JCB

4-chloro-2-methoxybenzoic acid C8H7ClO3[2, 3]

Compound Data



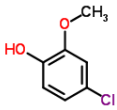
Melting point	**146.50 °C**	**419.65 K**			
CSID	84565	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	186.5924	**H bond donors**	1	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.35 g/cm^3
SMILES	O=C(O)c1c(OC)cc(Cl)cc1				
STD InChIKey	UFEYMXHWIHFRBX-UHFFFAOYAL				

Melting Points

mp °C	source
146.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
147.00	Alfa Aesar

4-chloro-2-methoxyphenol C7H7ClO2[3, 64]

Compound Data

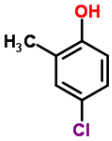


Melting point	**16.75 °C**	**289.90 K**			
CSID	26091	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.5823	**H bond donors**	1	**ACD/LogP**	2.36
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	Clc1cc(OC)c(O)cc1				
STD InChIKey	FVZQMMMRFNURSH-UHFFFAOYAH				

Melting Points

mp °C	source
17.00	Alfa Aesar
16.50	PHYSPROP

4-chloro-2-methylphenol C7H7ClO[2, 3, 64]



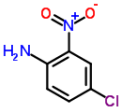
Compound Data

Melting point	**48.33 °C**	**321.48 K**			
CSID	14165	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	142.5829	**H bond donors**	1	**ACD/LogP**	2.89
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	Clc1cc(c(O)cc1)C				
STD InChIKey	RHPUJHQBPORFGV-UHFFFAOYAB				

Melting Points

mp °C	source
47.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
47.00	Alfa Aesar
51.00	PHYSPROP

4-chloro-2-nitroaniline C6H5ClN2O2[2, 3, 61, 64]



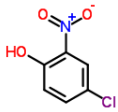
Compound Data

Melting point	**116.75 °C**	**389.90 K**			
CSID	6713	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.5691	**H bond donors**	2	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.49 g/cm^3
SMILES	Clc1cc([N+]([O-])=O)c(N)cc1				
STD InChIKey	PBGKNXWGYQPUJK-UHFFFAOYAL				

Melting Points

mp °C	source
118.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
116.00	Alfa Aesar
116.50	Oxford University MSDS
116.50	PHYSPROP

4-chloro-2-nitrophenol C6H4ClNO3[3, 48, 64]



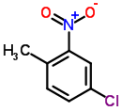
Compound Data

Melting point	**88.17 °C**	**361.32 K**			
CSID	6714	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	173.5539	**H bond donors**	1	**ACD/LogP**	2.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.55 g/cm^3
SMILES	Clc1cc([N+]([O-])=O)c(O)cc1				
STD InChIKey	NWSIFTLPLKCTSX-UHFFFAOYAR				

Melting Points

mp °C	source
87.00	Alfa Aesar
89.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
88.50	PHYSPROP

4-chloro-2-nitrotoluene C7H6ClNO2[2, 3, 64]



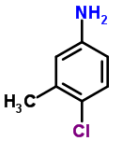
Compound Data

Melting point	**37.67 °C**	**310.82 K**			
CSID	6709	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	0	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	Clc1cc([N+]([O-])=O)c(cc1)C				
STD InChIKey	SQFLFRQWPBEDHM-UHFFFAOYAL				

Melting Points

mp °C	source
39.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
36.00	Alfa Aesar
38.00	PHYSPROP

4-chloro-3-methylaniline C7H8ClN[3, 64]



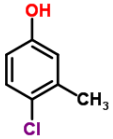
Compound Data

Melting point	**83.75 °C**	**356.90 K**			
CSID	22006	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	141.5981	**H bond donors**	2	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Clc1ccc(N)cc1C				
STD InChIKey	HIHCTGNZNHSZPP-UHFFFAOYAB				

Melting Points

mp °C	source
84.00	Alfa Aesar
83.50	PHYSPROP

4-chloro-3-methylphenol C7H7ClO[2, 3, 61, 64]



Compound Data

Melting point	**66.75 °C**	**339.90 K**			
CSID	21106018	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	142.5829	**H bond donors**	1	**ACD/LogP**	2.89
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	Oc1ccc(Cl)c(C)c1				
STD InChIKey	CFKMVGJGLGKFKI-UHFFFAOYAE				

Melting Points

mp °C	source
67.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
66.00	Alfa Aesar
67.00	Oxford University MSDS
67.00	PHYSPROP

4-chloro-3-nitroaniline C6H5ClN2O2[2, 3, 64]

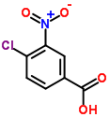
Compound Data

Melting point	**102.00 °C**	**375.15 K**			
CSID	11967	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.5691	**H bond donors**	2	**ACD/LogP**	1.98
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.49 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1Cl)N				
STD InChIKey	FOHHWGVAOVDVLP-UHFFFAOYAC				

Melting Points

mp °C	source
100.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
103.00	Alfa Aesar
103.00	PHYSPROP

4-chloro-3-nitrobenzoic acid C7H4ClNO4[3, 35, 64]



Compound Data

Melting point	**182.53 °C**	**455.68 K**			
CSID	7044	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	1	**ACD/LogP**	2.37
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1Cl)C(=O)O				
STD InChIKey	DFXQXFGFOLXAPO-UHFFFAOYAM				

Melting Points

mp °C	source
182.00	Alfa Aesar

182.80	EPISuite-ChemSpider
182.80	PHYSPROP

4-chloro-3-nitrobenzonitrile C7H3ClN2O2[3, 64]

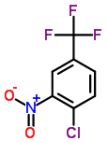
Compound Data

Melting point	**99.50 °C**	**372.65 K**			
CSID	13066	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.5639	**H bond donors**	0	**ACD/LogP**	1.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.48 g/cm^3
SMILES	c1cc(c(cc1C#N)[N+](=O)[O-])Cl				
STD InChIKey	XBLPHYSLHRGMNW-UHFFFAOYAQ				

Melting Points

mp °C	source
100.00	Alfa Aesar
99.00	PHYSPROP

4-chloro-3-nitrobenzotrifluoride C7H3ClF3NO2[3, 64]



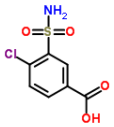
Compound Data

Melting point	**-2.75 °C**	**270.40 K**			
CSID	8151	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	225.5524	**H bond donors**	0	**ACD/LogP**	3.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	c1cc(c(cc1C(F)(F)F)[N+](=O)[O-])Cl				
STD InChIKey	TZGFQIXRVUHDLE-UHFFFAOYAM				

Melting Points

mp °C	source
-3.00	Alfa Aesar
-2.50	PHYSPROP

4-chloro-3-sulfamoylbenzoic acid C7H6ClNO4S[3, 64]



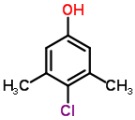
Compound Data

Melting point	**257.50 °C**	**530.65 K**			
CSID	13909	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	235.6448	**H bond donors**	3	**ACD/LogP**	0.92
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.65 g/cm^3
SMILES	O=S(=O)(c1cc(ccc1Cl)C(=O)O)N				
STD InChIKey	FHQAWINGVCDTTG-UHFFFAOYAK				

Melting Points

mp °C	source
258.00	Alfa Aesar
257.00	PHYSPROP

4-chloro-3,5-dimethylphenol C8H9ClO[2, 3, 61, 64]



Compound Data

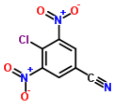
Melting point	**114.75 °C**	**387.90 K**			
CSID	21106017	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	156.6095	**H bond donors**	1	**ACD/LogP**	3.35
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Oc1cc(C)c(Cl)c(C)c1				
STD InChIKey	OSDLLIBGSJNGJE-UHFFFAOYAY				

Melting Points

mp °C	source
115.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
114.00	Alfa Aesar

115.00	Oxford University MSDS
115.00	PHYSPROP

4-chloro-3,5-dinitrobenzonitrile C7H2ClN3O4[3, 64]



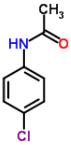
Compound Data

Melting point	**140.88 °C**	**414.02 K**			
CSID	15209	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	227.5615	**H bond donors**	0	**ACD/LogP**	0.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.68 g/cm^3
SMILES	O=[N+]([O-])c1cc(C#N)cc([N+]([O-])=O)c1Cl				
STD InChIKey	SCGDEDHSPCXGEC-UHFFFAOYAA				

Melting Points

mp °C	source
141.00	Alfa Aesar
140.75	PHYSPROP

4-chloroacetanilide C8H8ClNO[2, 3, 64]



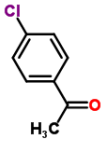
Compound Data

Melting point	**178.67 °C**	**451.82 K**			
CSID	10411	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	169.6082	**H bond donors**	1	**ACD/LogP**	2.05
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	Clc1ccc(NC(=O)C)cc1				
STD InChIKey	GGUOCFNAWIODMF-UHFFFAOYAH				

Melting Points

mp °C	source
178.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
179.00	Alfa Aesar
179.00	PHYSPROP

4-chloroacetophenone C8H7ClO[3, 31, 64]



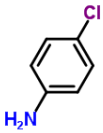
Compound Data

Melting point	**19.00 °C**	**292.15 K**			
CSID	13835126	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	154.5936	**H bond donors**	0	**ACD/LogP**	2.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	CC(=O)c1ccc(cc1)Cl				
STD InChIKey	BUZYGTVTZYSBCU-UHFFFAOYAU				

Melting Points

mp °C	source
19.00	Alfa Aesar
18.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
20.00	PHYSPROP

4-chloroaniline C6H6ClN[2, 3, 61, 64]



Compound Data

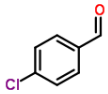
Melting point	**71.25 °C**	**344.40 K**			
CSID	13869339	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	127.5715	**H bond donors**	2	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	Nc1ccc(Cl)cc1				
STD InChIKey	QSNSCYSYFYORTR-UHFFFAOYAA				

Melting Points

mp °C	source

70.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
70.00	Alfa Aesar
72.50	Oxford University MSDS
72.50	PHYSPROP

4-chlorobenzaldehyde C7H5ClO[2, 3, 3, 61, 64]



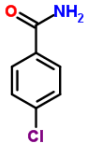
Compound Data

Melting point	**46.50 °C**	**319.65 K**			
CSID	21106019	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	140.567	**H bond donors**	0	**ACD/LogP**	2.21
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	c1cc(ccc1C=O)Cl				
STD InChIKey	AVPYQKSLYISFPO-UHFFFAOYAQ				

Melting Points

mp °C	source
46.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
46.00	Alfa Aesar
47.00	Alfa Aesar
46.00	Oxford University MSDS
47.50	PHYSPROP

4-chlorobenzamide C7H6ClNO[2, 3, 64]



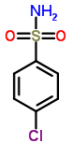
Compound Data

Melting point	**175.00 °C**	**448.15 K**			
CSID	11587	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	155.5816	**H bond donors**	2	**ACD/LogP**	1.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1ccc(Cl)cc1)N				
STD InChIKey	BLNVISNJTIRAHF-UHFFFAOYAB				

Melting Points

mp °C	source
173.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
178.00	Alfa Aesar
174.00	PHYSPROP

4-chlorobenzenesulfonamide C6H6ClNO2S[2, 3]



Compound Data

Melting point	**145.50 °C**	**418.65 K**			
CSID	60188	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.6353	**H bond donors**	2	**ACD/LogP**	0.84
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.47 g/cm^3
SMILES	O=S(=O)(c1ccc(Cl)cc1)N				
STD InChIKey	HHHDJHHNEURCNV-UHFFFAOYAK				

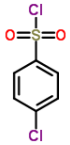
Melting Points

mp °C	source
145.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
146.00	Alfa Aesar

4-chlorobenzenesulfonyl chloride C6H4Cl2O2S[3, 64]

Compound Data

Melting point	**51.50 °C**	**324.65 K**			
CSID	7120	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	211.0658	**H bond donors**	0	**ACD/LogP**	2.84
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3



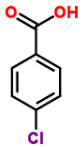
SMILES	O=S(Cl)(=O)c1ccc(Cl)cc1
STD InChIKey	ZLYBFBAHAQEEQQ-UHFFFAOYAF

Melting Points

mp °C	source
52.00	Alfa Aesar
51.00	PHYSPROP

4-chlorobenzoic acid C7H5ClO2[2, 3, 61, 64]

Compound Data



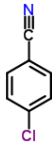
Melting point	**241.75 °C**	**514.90 K**			
CSID	6079	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.5664	**H bond donors**	1	**ACD/LogP**	2.65
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	O=C(O)c1ccc(Cl)cc1				
STD InChIKey	XRHGYUZYPHTUJZ-UHFFFAOYAE				

Melting Points

mp °C	source
240.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
241.00	Alfa Aesar
243.00	Oxford University MSDS
243.00	PHYSPROP

4-chlorobenzonitrile C7H4ClN[2, 3, 64]

Compound Data



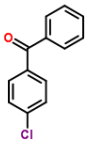
Melting point	**93.00 °C**	**366.15 K**			
CSID	11663	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	137.5664	**H bond donors**	0	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	c1cc(ccc1C#N)Cl				
STD InChIKey	GJNGXPDXRVXSEH-UHFFFAOYAB				

Melting Points

mp °C	source
92.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
92.00	Alfa Aesar
95.00	PHYSPROP

4-chlorobenzophenone C13H9ClO[2, 3, 64]

Compound Data

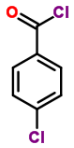


Melting point	**76.50 °C**	**349.65 K**			
CSID	8331	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	216.663	**H bond donors**	0	**ACD/LogP**	4.33
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	c1ccc(cc1)C(=O)c2ccc(cc2)Cl				
STD InChIKey	UGVRJVHOJNYEHR-UHFFFAOYAG				

Melting Points

mp °C	source
76.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
76.00	Alfa Aesar
77.50	PHYSPROP

4-chlorobenzoyl chloride C7H4Cl2O[3, 61, 64]



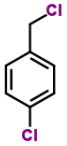
Compound Data

Melting point	**13.67 °C**	**286.82 K**			
CSID	8187	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.0121	**H bond donors**	0	**ACD/LogP**	2.97
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	O=C(Cl)c1ccc(Cl)cc1				
STD InChIKey	RKIDDEGICSMIJA-UHFFFAOYAV				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.00	Oxford University MSDS
16.00	PHYSPROP

4-chlorobenzyl chloride C7H6Cl2[2, 3, 64]



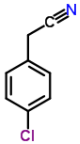
Compound Data

Melting point	**29.67 °C**	**302.82 K**			
CSID	7437	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	161.0285	**H bond donors**	0	**ACD/LogP**	3.08
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	ClCc1ccc(Cl)cc1				
STD InChIKey	JQZAEUFPPSRDOP-UHFFFAOYAV				

Melting Points

mp °C	source
30.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
28.00	Alfa Aesar
31.00	PHYSPROP

4-chlorobenzyl cyanide C8H6ClN[2, 3]



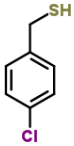
Compound Data

Melting point	**30.50 °C**	**303.65 K**			
CSID	211145	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	151.5929	**H bond donors**	0	**ACD/LogP**	2.04
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.19 g/cm^3
SMILES	Clc1ccc(cc1)CC#N				
STD InChIKey	IVYMIRMKXZAHRV-UHFFFAOYAK				

Melting Points

mp °C	source
31.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
30.00	Alfa Aesar

4-chlorobenzyl mercaptan C7H7ClS[2, 3, 64]



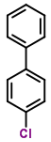
Compound Data

Melting point	**19.50 °C**	**292.65 K**			
CSID	72625	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	158.6485	**H bond donors**	0	**ACD/LogP**	3.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	Clc1ccc(cc1)CS				
STD InChIKey	GKQXPTHQTXCXEV-UHFFFAOYAX				

Melting Points

mp °C	source
19.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
20.00	Alfa Aesar
19.50	PHYSPROP

4-chlorobiphenyl C12H9Cl[7, 64]



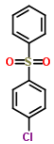
Compound Data

Melting point	**78.40 °C**	**351.55 K**			
CSID	15489	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	188.6529	**H bond donors**	0	**ACD/LogP**	4.55
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	Clc2ccc(c1ccccc1)cc2				
STD InChIKey	FPWNLURCHDRMHC-UHFFFAOYAG				

Melting Points

mp °C	source
78.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
78.80	PHYSPROP

4-chlorodiphenyl sulfone C12H9ClO2S[3, 64]



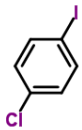
Compound Data

Melting point	**93.00 °C**	**366.15 K**			
CSID	6369	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	252.7167	**H bond donors**	0	**ACD/LogP**	3.30
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=S(=O)(c1ccc(Cl)cc1)c2ccccc2				
STD InChIKey	OFCFYWOKHPOXKF-UHFFFAOYAJ				

Melting Points

mp °C	source
92.00	Alfa Aesar
94.00	PHYSPROP

4-chloroiodobenzene C6H4ClI[2, 3, 64]



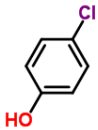
Compound Data

Melting point	**55.33 °C**	**328.48 K**			
CSID	13868660	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	238.4534	**H bond donors**	0	**ACD/LogP**	3.77
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.93 g/cm^3
SMILES	Ic1ccc(Cl)cc1				
STD InChIKey	GWQSENYKCGJTRI-UHFFFAOYAR				

Melting Points

mp °C	source
54.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
57.00	PHYSPROP

4-chlorophenol C6H5ClO[2, 3, 61, 64]



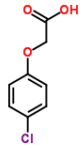
Compound Data

Melting point	**42.95 °C**	**316.10 K**			
CSID	13875219	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	128.5563	**H bond donors**	1	**ACD/LogP**	2.43
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Oc1ccc(Cl)cc1				
STD InChIKey	WXNZTHHGJRFXKQ-UHFFFAOYAX				

Melting Points

mp °C	source
44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
41.00	Alfa Aesar
44.00	Oxford University MSDS
42.80	PHYSPROP

4-chlorophenoxyacetic acid C8H7ClO3[3, 64]



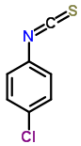
Compound Data

Melting point	**161.50 °C**	**434.65 K**			
CSID	24438	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	186.5924	**H bond donors**	1	**ACD/LogP**	2.03
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.37 g/cm^3
SMILES	Clc1ccc(OCC(=O)O)cc1				
STD InChIKey	SODPIMGUZLOIPE-UHFFFAOYAE				

Melting Points

mp °C	source
159.00	Alfa Aesar
164.00	PHYSPROP

4-chlorophenyl isothiocyanate C7H4ClNS[3, 64]



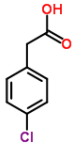
Compound Data

Melting point	**45.50 °C**	**318.65 K**			
CSID	15622	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	169.6314	**H bond donors**	0	**ACD/LogP**	3.91
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	Clc1ccc(\N=C=S)cc1				
STD InChIKey	MZZVFXMTZTVUFO-UHFFFAOYAL				

Melting Points

mp °C	source
45.00	Alfa Aesar
46.00	PHYSPROP

4-chlorophenylacetic acid C8H7ClO2[2, 3, 35, 64]



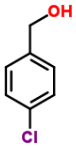
Compound Data

Melting point	**105.25 °C**	**378.40 K**			
CSID	15093	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	170.593	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	Clc1ccc(cc1)CC(=O)O				
STD InChIKey	CDPKJZJVTHSESZ-UHFFFAOYAC				

Melting Points

mp °C	source
103.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
105.00	Alfa Aesar
106.50	EPISuite-ChemSpider
106.50	PHYSPROP

4-chlorophenylmethanol C7H7ClO[2, 3, 61, 64]



Compound Data

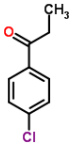
Melting point	**71.75 °C**	**344.90 K**			
CSID	12823	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	142.5829	**H bond donors**	1	**ACD/LogP**	1.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	Clc1ccc(cc1)CO				
STD InChIKey	PTHGDVCPCZKZKR-UHFFFAOYAC				

Melting Points

mp °C	source
71.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
70.00	Alfa Aesar
71.00	Oxford University MSDS

75.00	PHYSPROP

4-chloropropiophenone C9H9ClO[3, 47, 64]



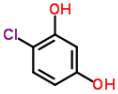
Compound Data

Melting point	**35.93 °C**	**309.08 K**			
CSID	21278	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	168.6202	**H bond donors**	0	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.13 g/cm^3
SMILES	O=C(c1ccc(Cl)cc1)CC				
STD InChIKey	ADCYRBXQAJXJTD-UHFFFAOYAE				

Melting Points

mp °C	source
35.00	Alfa Aesar
35.50	IUCr
37.30	PHYSPROP

4-chlororesorcinol C6H5ClO2[2, 3, 61, 64]



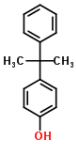
Compound Data

Melting point	**106.75 °C**	**379.90 K**			
CSID	1668	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.5557	**H bond donors**	2	**ACD/LogP**	1.67
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	Clc1ccc(O)cc1O				
STD InChIKey	JQVAPEJNIZULEK-UHFFFAOYAA				

Melting Points

mp °C	source
106.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
107.00	Alfa Aesar
107.00	Oxford University MSDS
107.00	PHYSPROP

4-cumylphenol C15H16O[2, 3, 61, 64]



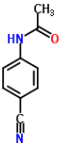
Compound Data

Melting point	**72.12 °C**	**345.27 K**			
CSID	11249	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	212.2869	**H bond donors**	1	**ACD/LogP**	4.17
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3
SMILES	Oc1ccc(cc1)C(c2ccccc2)(C)C				
STD InChIKey	QBDSZLJBMIMQRS-UHFFFAOYAW				

Melting Points

mp °C	source
70.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
72.00	Alfa Aesar
71.50	Oxford University MSDS
75.00	PHYSPROP

4-cyanoacetanilide C9H8N2O[3, 64]



Compound Data

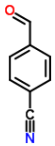
Melting point	**206.00 °C**	**479.15 K**			
CSID	34195	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	160.1726	**H bond donors**	1	**ACD/LogP**	1.37
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	O=C(Nc1ccc(C#N)cc1)C				
STD InChIKey	UFKRTEWFEYWIHD-UHFFFAOYAT				

Melting Points

mp °C	source
205.00	Alfa Aesar
207.00	PHYSPROP

4-cyanobenzaldehyde C8H5NO[2, 3, 64]

Compound Data



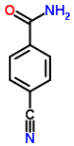
Melting point	**101.17 °C**	**374.32 K**			
CSID	59433	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	131.1314	**H bond donors**	0	**ACD/LogP**	1.30
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	N#Cc1ccc(C=O)cc1				
STD InChIKey	WZWIQYMTQZCSKI-UHFFFAOYAA				

Melting Points

mp °C	source
102.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
101.00	Alfa Aesar
100.50	PHYSPROP

4-cyanobenzamide C8H6N2O[3, 7]

Compound Data



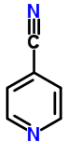
Melting point	**225.50 °C**	**498.65 K**			
CSID	68899	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	146.146	**H bond donors**	2	**ACD/LogP**	0.48
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	N#Cc1ccc(C(=O)N)cc1				
STD InChIKey	FUKWTMJZHKZKFA-UHFFFAOYAG				

Melting Points

mp °C	source
227.00	Alfa Aesar
224.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-cyanopyridine C6H4N2[3, 61, 64]

Compound Data



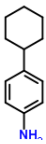
Melting point	**77.67 °C**	**350.82 K**			
CSID	7225	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	104.1094	**H bond donors**	0	**ACD/LogP**	0.41
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.12 g/cm^3
SMILES	N#Cc1ccncc1				
STD InChIKey	GPHQHTOMRSGBNZ-UHFFFAOYAF				

Melting Points

mp °C	source
78.00	Alfa Aesar
76.00	Oxford University MSDS
79.00	PHYSPROP

4-cyclohexylaniline C12H17N[2, 3, 64]

Compound Data



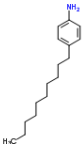
Melting point	**53.83 °C**	**326.98 K**			
CSID	72918	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.2701	**H bond donors**	2	**ACD/LogP**	3.46
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.01 g/cm^3
SMILES	c1cc(ccc1N)C2CCCCC2				
STD InChIKey	JLNMBIKJQAKQBH-UHFFFAOYAC				

Melting Points

mp °C	source
53.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
54.50	PHYSPROP

4-decylaniline C16H27N[3, 64]

Compound Data



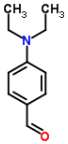
Melting point	**24.50 °C**	**297.65 K**			
CSID	83338	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	233.3923	**H bond donors**	2	**ACD/LogP**	6.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	0.91 g/cm^3
SMILES	Nc1ccc(cc1)CCCCCCCCCC				
STD InChIKey	WGENWPANMZLPIH-UHFFFAOYAC				

Melting Points

mp °C	source
24.00	Alfa Aesar
25.00	PHYSPROP

4-diethylaminobenzaldehyde C11H15NO[2, 3, 64]

Compound Data



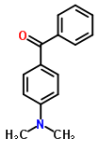
Melting point	**40.33 °C**	**313.48 K**			
CSID	60462	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	177.2429	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.03 g/cm^3
SMILES	O=Cc1ccc(N(CC)CC)cc1				
STD InChIKey	MNFZZNNFORDXSV-UHFFFAOYAA				

Melting Points

mp °C	source
40.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
40.00	Alfa Aesar
41.00	PHYSPROP

4-dimethylaminobenzophenone C15H15NO[3, 64]

Compound Data



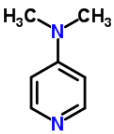
Melting point	**90.75 °C**	**363.90 K**			
CSID	10284	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	225.2857	**H bond donors**	0	**ACD/LogP**	3.52
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(c1ccc(N(C)C)cc1)c2ccccc2				
STD InChIKey	BEUGBYXJXMVRFO-UHFFFAOYAL				

Melting Points

mp °C	source
89.00	Alfa Aesar
92.50	PHYSPROP

4-dimethylaminopyridine C7H10N2[3, 61, 64]

Compound Data



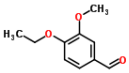
Melting point	**111.67 °C**	**384.82 K**			
CSID	13646	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1677	**H bond donors**	0	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	n1ccc(N(C)C)cc1				
STD InChIKey	VHYFNPMBLIVWCW-UHFFFAOYAL				

Melting Points

mp °C	source
112.00	Alfa Aesar
111.00	Oxford University MSDS
112.00	PHYSPROP

4-ethoxy-3-methoxybenzaldehyde C10H12O3[3, 64]

Compound Data



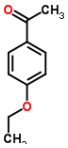
Melting point	**62.75 °C**	**335.90 K**			
CSID	60464	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	0	**ACD/LogP**	2.14
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	O=Cc1cc(OC)c(OCC)cc1				
STD InChIKey	BERFDQAMXIBOHM-UHFFFAOYAQ				

Melting Points

mp °C	source
61.00	Alfa Aesar
64.50	PHYSPROP

4-ethoxyacetophenone C10H12O2[3, 7]

Compound Data



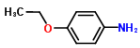
Melting point	**38.00 °C**	**311.15 K**			
CSID	65704	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	0	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.02 g/cm^3
SMILES	O=C(c1ccc(OCC)cc1)C				
STD InChIKey	YJFNFQHMQJCPRG-UHFFFAOYAX				

Melting Points

mp °C	source
37.00	Alfa Aesar
39.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-ethoxyaniline C8H11NO[2, 3, 61, 64]

Compound Data



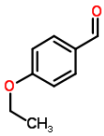
Melting point	**3.10 °C**	**276.25 K**			
CSID	21106155	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	137.179	**H bond donors**	2	**ACD/LogP**	1.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.04 g/cm^3
SMILES	CCOc1ccc(N)cc1				
STD InChIKey	IMPPGHMHELILKG-UHFFFAOYAH				

Melting Points

mp °C	source
4.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
3.00	Alfa Aesar
3.00	Oxford University MSDS
2.40	PHYSPROP

4-ethoxybenzaldehyde C9H10O2[2, 3, 64]

Compound Data



Melting point	**13.83 °C**	**286.98 K**			
CSID	21105889	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	0	**ACD/LogP**	2.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.06 g/cm^3
SMILES	CCOc1ccc(cc1)C=O				

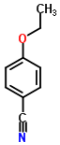
STD InChIKey	JRHHJNMASOIRDS-UHFFFAOYAT

Melting Points

mp °C	source
14.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
14.00	Alfa Aesar
13.50	PHYSPROP

4-ethoxybenzonitrile C9H9NO[3, 64]

Compound Data



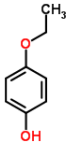
Melting point	**61.75 °C**	**334.90 K**			
CSID	124526	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	147.1739	**H bond donors**	0	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	N#Cc1ccc(OCC)cc1				
STD InChIKey	PJRLUGQMEZZDIY-UHFFFAOYAE				

Melting Points

mp °C	source
62.00	Alfa Aesar
61.50	PHYSPROP

4-ethoxyphenol C8H10O2[3, 64]

Compound Data



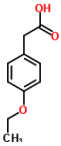
Melting point	**66.25 °C**	**339.40 K**			
CSID	11651	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	1	**ACD/LogP**	1.86
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	CCOc1ccc(cc1)O				
STD InChIKey	LKVFCSWBKOVHAH-UHFFFAOYAY				

Melting Points

mp °C	source
66.00	Alfa Aesar
66.50	PHYSPROP

4-ethoxyphenylacetic acid C10H12O3[3, 64]

Compound Data



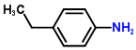
Melting point	**88.75 °C**	**361.90 K**			
CSID	70988	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	1	**ACD/LogP**	1.95
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.14 g/cm^3
SMILES	O=C(O)Cc1ccc(OCC)cc1				
STD InChIKey	ZVVWZNFSMIFGEP-UHFFFAOYAB				

Melting Points

mp °C	source
89.00	Alfa Aesar
88.50	PHYSPROP

4-ethylaniline C8H11N[3, 31, 64]

Compound Data



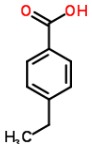
Melting point	**-4.93 °C**	**268.22 K**			
CSID	21106525	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	CCc1ccc(N)cc1				
STD InChIKey	HRXZRAXKKNUKRF-UHFFFAOYAA				

Melting Points

mp °C	source
-5.00	Alfa Aesar
-5.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-4.80	PHYSPROP

4-ethylbenzoic acid C9H10O2[3, 64]

Compound Data



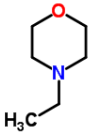
Melting point	**112.75 °C**	**385.90 K**			
CSID	11589	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	2.89
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	O=C(O)c1ccc(cc1)CC				
STD InChIKey	ZQVKTHRQIXSMGY-UHFFFAOYAV				

Melting Points

mp °C	source
113.00	Alfa Aesar
112.50	PHYSPROP

4-ethylmorpholine C6H13NO[3, 61, 64]

Compound Data



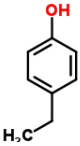
Melting point	**-63.33 °C**	**209.82 K**			
CSID	7244	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	115.1735	**H bond donors**	0	**ACD/LogP**	0.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.91 g/cm^3
SMILES	O1CCN(CC)CC1				
STD InChIKey	HVCNXQOWACZAFN-UHFFFAOYAU				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-63.00	Oxford University MSDS
-64.00	PHYSPROP

4-ethylphenol C8H10O[3, 31, 61, 64]

Compound Data



Melting point	**44.62 °C**	**317.77 K**			
CSID	28982	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	2.47
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.01 g/cm^3
SMILES	Oc1ccc(cc1)CC				
STD InChIKey	HXDOZKJGKXYMEW-UHFFFAOYAF				

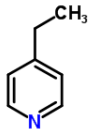
Melting Points

mp °C	source
43.00	Alfa Aesar
47.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
43.50	Oxford University MSDS
45.00	PHYSPROP

4-ethylpyridine C7H9N[3, 64]

Compound Data

Melting point	**-90.75 °C**	**182.40 K**			
CSID	21106560	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	0	**ACD/LogP**	1.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.93 g/cm^3



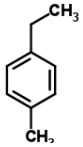
SMILES	CCc1ccncc1
STD InChIKey	VJXRKZJMGVSXPX-UHFFFAOYAD

Melting Points

mp °C	source
-91.00	Alfa Aesar
-90.50	PHYSPROP

4-ethyltoluene C9H12[3, 4, 64]

Compound Data



Melting point	**-62.10 °C**	**211.05 K**			
CSID	11660	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.1916	**H bond donors**	0	**ACD/LogP**	3.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	c1cc(ccc1CC)C				
STD InChIKey	JRLPEMVDPFPYPJ-UHFFFAOYAO				

Melting Points

mp °C	source
-62.00	Alfa Aesar
-62.00	American Petroleum Institute. Research Project 44; Selected ...
-62.30	PHYSPROP

4-fluoro-2-nitrophenol C6H4FNO3[3, 48]

Compound Data

Melting point	**74.00 °C**	**347.15 K**			
CSID	120011	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	157.0993	**H bond donors**	1	**ACD/LogP**	1.90
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.51 g/cm^3
SMILES	O=[N+]([O-])c1cc(F)ccc1O				
STD InChIKey	ZHRLVDHMIJDWSS-UHFFFAOYAS				

Melting Points

mp °C	source
75.00	Alfa Aesar
73.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

4-fluoro-2-nitrotoluene C7H6FNO2[3, 64]

Compound Data

Melting point	**26.50 °C**	**299.65 K**			
CSID	61280	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	155.1264	**H bond donors**	0	**ACD/LogP**	2.36
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	Fc1cc([N+]([O-])=O)c(cc1)C				
STD InChIKey	SKWTUNAAJNDEIK-UHFFFAOYAG				

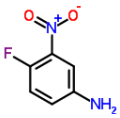
Melting Points

mp °C	source
26.00	Alfa Aesar
27.00	PHYSPROP

4-fluoro-3-nitroaniline C6H5FN2O2[3, 64]

Compound Data

Melting point	**96.75 °C**	**369.90 K**



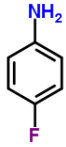
CSID	61087	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	156.1145	**H bond donors**	2	**ACD/LogP**	1.27
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.45 g/cm^3
SMILES	O=[N+]([O-])c1c(F)ccc(N)c1				
STD InChIKey	LLIOADBCFIXIEU-UHFFFAOYAJ				

Melting Points

mp °C	source
96.00	Alfa Aesar
97.50	PHYSPROP

4-fluoroaniline C6H6FN[3, 64]

Compound Data



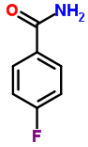
Melting point	**-1.40 °C**	**271.75 K**			
CSID	9349	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	111.1169	**H bond donors**	2	**ACD/LogP**	1.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	Fc1ccc(N)cc1				
STD InChIKey	KRZCOLNOCZKSDF-UHFFFAOYAY				

Melting Points

mp °C	source
-2.00	Alfa Aesar
-0.80	PHYSPROP

4-fluorobenzamide C7H6FNO[3, 64]

Compound Data



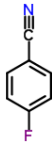
Melting point	**155.75 °C**	**428.90 K**			
CSID	64644	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	139.127	**H bond donors**	2	**ACD/LogP**	0.91
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	O=C(c1ccc(F)cc1)N				
STD InChIKey	VNDHYTGVCGVETQ-UHFFFAOYAF				

Melting Points

mp °C	source
156.00	Alfa Aesar
155.50	PHYSPROP

4-fluorobenzonitrile C7H4FN[3, 64]

Compound Data



Melting point	**35.40 °C**	**308.55 K**			
CSID	13861	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1118	**H bond donors**	0	**ACD/LogP**	1.70
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.15 g/cm^3
SMILES	N#Cc1ccc(F)cc1				
STD InChIKey	AEKVBBNGWBBYLL-UHFFFAOYAJ				

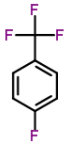
Melting Points

mp °C	source
36.00	Alfa Aesar
34.80	PHYSPROP

4-fluorobenzotrifluoride C7H4F4[3, 64]

Compound Data

Melting point	**-41.85 °C**	**231.30 K**			
CSID	61190	**H bond acceptors**	0	**Rule of 5 violations**	0



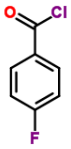
Molecular weight	164.1003	**H bond donors**	0	**ACD/LogP**	2.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	FC(F)(F)c1ccc(F)cc1				
STD InChIKey	UNNNAIWPDLRVRN-UHFFFAOYAF				

Melting Points

mp °C	source
-42.00	Alfa Aesar
-41.70	PHYSPROP

4-fluorobenzoyl chloride C7H4ClFO[3, 64]

Compound Data



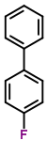
Melting point	**9.50 °C**	**282.65 K**			
CSID	61196	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	158.5575	**H bond donors**	0	**ACD/LogP**	2.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	O=C(Cl)c1ccc(F)cc1				
STD InChIKey	CZKLEJHVLCMVQR-UHFFFAOYAL				

Melting Points

mp °C	source
10.00	Alfa Aesar
9.00	PHYSPROP

4-fluorobiphenyl C12H9F[3, 64]

Compound Data



Melting point	**74.10 °C**	**347.25 K**			
CSID	9089	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	172.1983	**H bond donors**	0	**ACD/LogP**	3.91
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	Fc2ccc(c1ccccc1)cc2				
STD InChIKey	RUYZJEIKQYLEGZ-UHFFFAOYAQ				

Melting Points

mp °C	source
74.00	Alfa Aesar
74.20	PHYSPROP

4-fluorophenol C6H5FO[3, 61, 64, 72, 72]

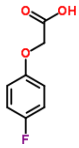
Compound Data

Melting point	**46.10 °C**	**319.25 K**			
CSID	9350	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	112.1017	**H bond donors**	1	**ACD/LogP**	1.77
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	Fc1ccc(O)cc1				
STD InChIKey	RHMPLDJJXGPMEX-UHFFFAOYAV				

Melting Points

mp °C	source
46.00	Alfa Aesar
45.50	Oxford University MSDS
48.00	PHYSPROP
44.50	Sigma-Aldrich
46.50	Sigma-Aldrich

4-fluorophenoxyacetic acid C8H7FO3[3, 64]



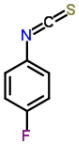
Compound Data

Melting point	**104.62 °C**	**377.77 K**			
CSID	61199	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	170.1378	**H bond donors**	1	**ACD/LogP**	1.47
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	Fc1ccc(OCC(=O)O)cc1				
STD InChIKey	ZBIULCVFFJJYTN-UHFFFAOYAV				

Melting Points

mp °C	source
105.00	Alfa Aesar
104.25	PHYSPROP

4-fluorophenyl isothiocyanate C7H4FNS[3, 64]



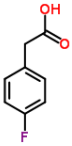
Compound Data

Melting point	**26.50 °C**	**299.65 K**			
CSID	14507	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	153.1768	**H bond donors**	0	**ACD/LogP**	3.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	Fc1ccc(\N=C=S)cc1				
STD InChIKey	NFIUJHJMCQQYDL-UHFFFAOYAS				

Melting Points

mp °C	source
26.00	Alfa Aesar
27.00	PHYSPROP

4-fluorophenylacetic acid C8H7FO2[3, 64]



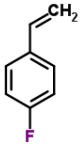
Compound Data

Melting point	**84.50 °C**	**357.65 K**			
CSID	9454	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	154.1384	**H bond donors**	1	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	Fc1ccc(cc1)CC(=O)O				
STD InChIKey	MGKPFALCNDRSQD-UHFFFAOYAI				

Melting Points

mp °C	source
83.00	Alfa Aesar
86.00	PHYSPROP

4-fluorostyrene C8H7F[3, 64]



Compound Data

Melting point	**-35.25 °C**	**237.90 K**			
CSID	61200	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	122.1396	**H bond donors**	0	**ACD/LogP**	2.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.02 g/cm^3
SMILES	Fc1ccc(\C=C)cc1				
STD InChIKey	JWVTWJNGILGLAT-UHFFFAOYAH				

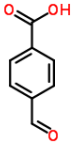
Melting Points

mp °C	source
-36.00	Alfa Aesar
-34.50	PHYSPROP

4-formylbenzoic acid C8H6O3[2, 3]

Compound Data

Melting point	**246.00 °C**	**519.15 K**



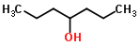
CSID	11591	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1314	**H bond donors**	1	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)c1ccc(C=O)cc1				
STD InChIKey	GOUHYARYYWKXHS-UHFFFAOYAP				

Melting Points

mp °C	source
247.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
245.00	Alfa Aesar

4-heptanol C7H16O[64, 82]

Compound Data



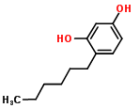
Melting point	**-41.60 °C**	**231.55 K**			
CSID	11029	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	116.2013	**H bond donors**	1	**ACD/LogP**	2.29
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.82 g/cm^3
SMILES	OC(CCC)CCC				
STD InChIKey	YVBCULSIZWMTFY-UHFFFAOYAT				

Melting Points

mp °C	source
-41.20	PHYSPROP
-42.00	Wilhoit R. C. Physical and Thermodynamic Properties of Aliph...

4-hexylbenzene-1,3-diol C12H18O2[3, 61, 64]

Compound Data



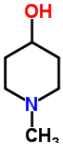
Melting point	**66.33 °C**	**339.48 K**			
CSID	21106121	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	194.2701	**H bond donors**	2	**ACD/LogP**	3.88
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.05 g/cm^3
SMILES	Oc1cc(O)ccc1CCCCCC				
STD InChIKey	WFJIVOKAWHGMBH-UHFFFAOYAH				

Melting Points

mp °C	source
66.00	Alfa Aesar
65.00	Oxford University MSDS
68.00	PHYSPROP

4-hydroxy-1-methylpiperidine C6H13NO[3, 64]

Compound Data



Melting point	**28.50 °C**	**301.65 K**			
CSID	59438	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	115.1735	**H bond donors**	1	**ACD/LogP**	-0.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	OC1CCN(C)CC1				
STD InChIKey	BAUWRHPMUVYFOD-UHFFFAOYAG				

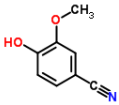
Melting Points

mp °C	source
28.00	Alfa Aesar
29.00	PHYSPROP

4-hydroxy-3-methoxybenzonitrile C8H7NO2[3, 64]

Compound Data

Melting point	**86.50 °C**	**359.65 K**	



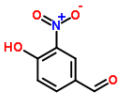
CSID	70511	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	149.1467	**H bond donors**	1	**ACD/LogP**	1.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	N#Cc1cc(OC)c(O)cc1				
STD InChIKey	QJRWLNLUIAJTAD-UHFFFAOYAP				

Melting Points

mp °C	source
87.00	Alfa Aesar
86.00	PHYSPROP

4-hydroxy-3-nitrobenzaldehyde C7H5NO4[3, 64]

Compound Data



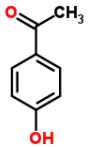
Melting point	**141.50 °C**	**414.65 K**			
CSID	17162	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	167.1189	**H bond donors**	1	**ACD/LogP**	2.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.50 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1O)C=O				
STD InChIKey	YTHJCZRFJGXPTL-UHFFFAOYAA				

Melting Points

mp °C	source
142.00	Alfa Aesar
141.00	PHYSPROP

4-hydroxyacetophenone C8H8O2[2, 3, 64]

Compound Data



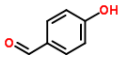
Melting point	**108.17 °C**	**381.32 K**			
CSID	7189	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	1	**ACD/LogP**	1.42
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(c1ccc(O)cc1)C				
STD InChIKey	TXFPEBPIARQUIG-UHFFFAOYAU				

Melting Points

mp °C	source
108.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
107.00	Alfa Aesar
109.50	PHYSPROP

4-hydroxybenzaldehyde C7H6O2[3, 3, 64]

Compound Data



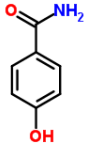
Melting point	**117.33 °C**	**390.48 K**			
CSID	123	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1213	**H bond donors**	1	**ACD/LogP**	1.39
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=Cc1ccc(O)cc1				
STD InChIKey	RGHHSNMVTDWUBI-UHFFFAOYAN				

Melting Points

mp °C	source
118.00	Alfa Aesar
117.00	Alfa Aesar
117.00	PHYSPROP

4-hydroxybenzamide C7H7NO2[2, 3, 64]

Compound Data



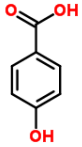
Melting point	**161.17 °C**	**434.32 K**			
CSID	58563	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	3	**ACD/LogP**	0.25
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1ccc(O)cc1)N				
STD InChIKey	QXSAKPUBHTZHKW-UHFFFAOYAO				

Melting Points

mp °C	source
161.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
161.00	Alfa Aesar
161.50	PHYSPROP

4-hydroxybenzoic acid C7H6O3[2, 3, 35, 64]

Compound Data



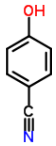
Melting point	**215.25 °C**	**488.40 K**			
CSID	132	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	138.1207	**H bond donors**	2	**ACD/LogP**	1.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.38 g/cm^3
SMILES	c1cc(ccc1C(=O)O)O				
STD InChIKey	FJKROLUGYXJWQN-UHFFFAOYAQ				

Melting Points

mp °C	source
217.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
215.00	Alfa Aesar
214.50	EPISuite-ChemSpider
214.50	PHYSPROP

4-hydroxybenzonitrile C7H5NO[2, 3, 61, 64]

Compound Data



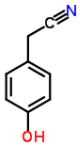
Melting point	**111.75 °C**	**384.90 K**			
CSID	12478	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	119.1207	**H bond donors**	1	**ACD/LogP**	1.60
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	N#Cc1ccc(O)cc1				
STD InChIKey	CVNOWLNNPYYEOH-UHFFFAOYAK				

Melting Points

mp °C	source
112.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
112.00	Alfa Aesar
111.50	Oxford University MSDS
111.50	PHYSPROP

4-hydroxybenzyl cyanide C8H7NO[2, 3, 7]

Compound Data

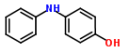


Melting point	**69.67 °C**	**342.82 K**			
CSID	24729	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	133.1473	**H bond donors**	1	**ACD/LogP**	0.71
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	N#CCc1ccc(O)cc1				
STD InChIKey	AYKYOOPFBCOXSL-UHFFFAOYAG				

Melting Points

mp °C	source
71.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
69.00	Alfa Aesar
69.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-hydroxydiphenylamine C12H11NO[3, 64]



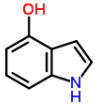
Compound Data

Melting point	**71.00 °C**	**344.15 K**			
CSID	21111849	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	185.2218	**H bond donors**	2	**ACD/LogP**	2.82
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.20 g/cm^3
SMILES	Oc2ccc(Nc1ccccc1)cc2				
STD InChIKey	JTTMYKSFKOOQLP-UHFFFAOYAT				

Melting Points

mp °C	source
69.00	Alfa Aesar
73.00	PHYSPROP

4-hydroxyindole C8H7NO[3, 64]



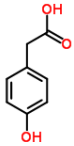
Compound Data

Melting point	**99.00 °C**	**372.15 K**			
CSID	67953	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	133.1473	**H bond donors**	2	**ACD/LogP**	1.41
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	c1cc2c(cc[nH]2)c(c1)O				
STD InChIKey	NLMQHXUGJIAKTH-UHFFFAOYAU				

Melting Points

mp °C	source
98.00	Alfa Aesar
100.00	PHYSPROP

4-hydroxyphenylacetic acid C8H8O3[3, 35, 64]



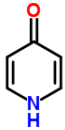
Compound Data

Melting point	**151.00 °C**	**424.15 K**			
CSID	124	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	O=C(O)Cc1ccc(O)cc1				
STD InChIKey	XQXPVVBIMDBYFF-UHFFFAOYAR				

Melting Points

mp °C	source
149.00	Alfa Aesar
152.00	EPISuite-ChemSpider
152.00	PHYSPROP

4-hydroxypyridine C5H5NO[3, 64]



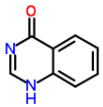
Compound Data

Melting point	**147.40 °C**	**420.55 K**			
CSID	11787	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	95.0993	**H bond donors**	1	**ACD/LogP**	-0.99
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	O=C\1\C=C/N/C=C/1				
STD InChIKey	GCNTZFIIOFTKIY-UHFFFAOYAB				

Melting Points

mp °C	source
145.00	Alfa Aesar
149.80	PHYSPROP

4-hydroxyquinazoline C8H6N2O[3, 64]



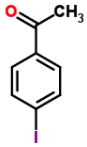
Compound Data

Melting point	**217.75 °C 490.90 K**				
CSID	56797	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	146.146	**H bond donors**	1	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.31 g/cm^3
SMILES	O=C2\N=C/Nc1ccccc12				
STD InChIKey	QMNUDYFKZYBWQX-UHFFFAOYAB				

Melting Points

mp °C	source
218.00	Alfa Aesar
217.50	PHYSPROP

4-iodoacetophenone C8H7IO[3, 47, 47, 64]



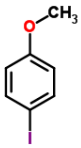
Compound Data

Melting point	**84.80 °C 357.95 K**				
CSID	65701	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	246.045	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.72 g/cm^3
SMILES	O=C(c1ccc(I)cc1)C				
STD InChIKey	JZJWCDQGIPQBAO-UHFFFAOYAH				

Melting Points

mp °C	source
83.00	Alfa Aesar
84.85	IUCr
85.35	IUCr
86.00	PHYSPROP

4-iodoanisole C7H7IO[2, 3, 64]



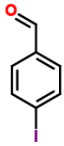
Compound Data

Melting point	**51.00 °C 324.15 K**				
CSID	62877	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	234.0343	**H bond donors**	0	**ACD/LogP**	3.39
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.73 g/cm^3
SMILES	Ic1ccc(OC)cc1				
STD InChIKey	SYSZENVIJHPFNL-UHFFFAOYAO				

Melting Points

mp °C	source
50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
50.00	Alfa Aesar
53.00	PHYSPROP

4-iodobenzaldehyde C7H5IO[3, 7]



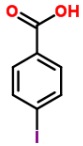
Compound Data

Melting point	**77.50 °C 350.65 K**				
CSID	87265	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	232.0185	**H bond donors**	0	**ACD/LogP**	2.83
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.88 g/cm^3
SMILES	O=Cc1ccc(I)cc1				
STD InChIKey	NIEBHDXUIJSHSL-UHFFFAOYAV				

Melting Points

mp °C	source
77.00	Alfa Aesar
78.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-iodobenzoic acid $C_7H_5IO_2$[2, 35, 64]



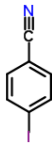
Compound Data

Melting point	**271.00 °C**	**544.15 K**			
CSID	11588	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	248.0179	**H bond donors**	1	**ACD/LogP**	3.02
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.00 g/cm^3
SMILES	O=C(O)c1ccc(I)cc1				
STD InChIKey	GHICCUXQJBDNRN-UHFFFAOYAH				

Melting Points

mp °C	source
273.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
270.00	EPISuite-ChemSpider
270.00	PHYSPROP

4-iodobenzonitrile C_7H_4IN[3, 7]



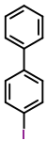
Compound Data

Melting point	**125.50 °C**	**398.65 K**			
CSID	68939	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	229.0178	**H bond donors**	0	**ACD/LogP**	2.68
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.91 g/cm^3
SMILES	N#Cc1ccc(I)cc1				
STD InChIKey	XOKDXPVXJWTSRM-UHFFFAOYAU				

Melting Points

mp °C	source
126.00	Alfa Aesar
125.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-iodobiphenyl $C_{12}H_9I$[3, 7, 64]



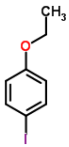
Compound Data

Melting point	**113.17 °C**	**386.32 K**			
CSID	14585	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	280.1043	**H bond donors**	0	**ACD/LogP**	5.18
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.58 g/cm^3
SMILES	Ic2ccc(c1ccccc1)cc2				
STD InChIKey	NXYICUMSYKIABQ-UHFFFAOYAY				

Melting Points

mp °C	source
112.00	Alfa Aesar
114.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
113.50	PHYSPROP

4-iodophenetole C_8H_9IO[3, 64]



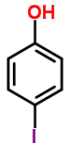
Compound Data

Melting point	**28.50 °C**	**301.65 K**			
CSID	191427	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	248.0609	**H bond donors**	0	**ACD/LogP**	3.92
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.63 g/cm^3
SMILES	Ic1ccc(OCC)cc1				
STD InChIKey	VSIIHWOJPSSIDI-UHFFFAOYAA				

Melting Points

mp °C	source
28.00	Alfa Aesar
29.00	PHYSPROP

4-iodophenol C_6H_5IO[2, 3, 61, 64]



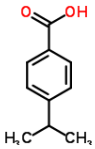
Compound Data

Melting point	**93.12 °C**	**366.27 K**			
CSID	10432	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	220.0078	**H bond donors**	1	**ACD/LogP**	2.99
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.00 g/cm^3
SMILES	c1cc(ccc1O)I				
STD InChIKey	VSMDINRNYYEDRN-UHFFFAOYAR				

Melting Points

mp °C	source
94.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
93.00	Alfa Aesar
92.00	Oxford University MSDS
93.50	PHYSPROP

4-isopropylbenzoic acid $C_{10}H_{12}O_2$[3, 64]



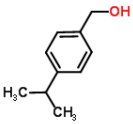
Compound Data

Melting point	**118.25 °C**	**391.40 K**			
CSID	10363	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	1	**ACD/LogP**	3.23
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.08 g/cm^3
SMILES	O=C(O)c1ccc(cc1)C(C)C				
STD InChIKey	CKMXAIVXVKGGFM-UHFFFAOYAY				

Melting Points

mp °C	source
119.00	Alfa Aesar
117.50	PHYSPROP

4-isopropylbenzyl alcohol $C_{10}H_{14}O$[3, 64]



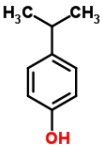
Compound Data

Melting point	**27.50 °C**	**300.65 K**			
CSID	21105932	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	1	**ACD/LogP**	2.37
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.98 g/cm^3
SMILES	OCc1ccc(cc1)C(C)C				
STD InChIKey	OIGWAXDAPKFNCQ-UHFFFAOYAM				

Melting Points

mp °C	source
27.00	Alfa Aesar
28.00	PHYSPROP

4-isopropylphenol $C_9H_{12}O$[2, 2, 3, 64, 72]



Compound Data

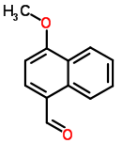
Melting point	**60.66 °C**	**333.81 K**			
CSID	7185	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	1	**ACD/LogP**	2.82
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	Oc1ccc(cc1)C(C)C				
STD InChIKey	YQUQWHNMBPIWGK-UHFFFAOYAX				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
61.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
60.00	Alfa Aesar

62.30	PHYSPROP
60.00	Sigma-Aldrich

4-methoxy-1-naphthaldehyde C12H10O2[3, 64]



Compound Data

Melting point	**34.40 °C**	**307.55 K**			
CSID	76852	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	0	**ACD/LogP**	2.93
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=Cc2c1ccccc1c(OC)cc2				
STD InChIKey	MVXMNHYVCLMLDD-UHFFFAOYAE				

Melting Points

mp °C	source
34.00	Alfa Aesar
34.80	PHYSPROP

4-methoxy-2-nitroaniline C7H8N2O3[3, 64]

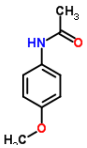
Compound Data

Melting point	**125.50 °C**	**398.65 K**			
CSID	60158	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	168.15	**H bond donors**	2	**ACD/LogP**	1.94
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.32 g/cm^3
SMILES	[O-][N+](=O)c1c(ccc(OC)c1)N				
STD InChIKey	QFMJFXFXQAFGBO-UHFFFAOYAL				

Melting Points

mp °C	source
127.00	Alfa Aesar
124.00	PHYSPROP

4-methoxyacetanilide C9H11NO2[3, 64]



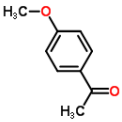
Compound Data

Melting point	**129.00 °C**	**402.15 K**			
CSID	5622	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	165.1891	**H bond donors**	1	**ACD/LogP**	1.09
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.13 g/cm^3
SMILES	O=C(Nc1ccc(OC)cc1)C				
STD InChIKey	XVAIDCNLVLTVFM-UHFFFAOYAL				

Melting Points

mp °C	source
127.00	Alfa Aesar
131.00	PHYSPROP

4-methoxyacetophenone C9H10O2[2, 3, 64]



Compound Data

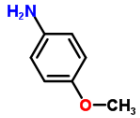
Melting point	**38.17 °C**	**311.32 K**			
CSID	13835344	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	0	**ACD/LogP**	1.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	COc1ccc(cc1)C(C)=O				
STD InChIKey	NTPLXRHDUXRPNE-UHFFFAOYAX				

Melting Points

mp °C	source
38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
38.00	Alfa Aesar

38.50	PHYSPROP

4-methoxyaniline C7H9NO[2, 3, 61, 64]



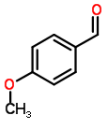
Compound Data

Melting point	**57.80 °C**	**330.95 K**			
CSID	13869414	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	123.1525	**H bond donors**	2	**ACD/LogP**	0.94
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	COc1ccc(cc1)N				
STD InChIKey	BHAAPTBBJKJZER-UHFFFAOYAR				

Melting Points

mp °C	source
59.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
58.00	Alfa Aesar
57.00	Oxford University MSDS
57.20	PHYSPROP

4-methoxybenzaldehyde C8H8O2[2, 3, 3, 64]



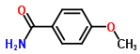
Compound Data

Melting point	**0.25 °C**	**273.40 K**			
CSID	21105937	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	0	**ACD/LogP**	1.70
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	COc1ccc(C=O)cc1				
STD InChIKey	ZRSNZINYAWTAHE-UHFFFAOYAA				

Melting Points

mp °C	source
-1.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
1.00	Alfa Aesar
1.00	Alfa Aesar
0.00	PHYSPROP

4-methoxybenzamide C8H9NO2[2, 3, 64]



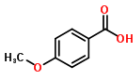
Compound Data

Melting point	**165.83 °C**	**438.98 K**			
CSID	10256859	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	0.81
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	COc1ccc(cc1)C(N)=O				
STD InChIKey	GUCPYIYFQVTFSI-UHFFFAOYAG				

Melting Points

mp °C	source
165.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
166.00	Alfa Aesar
166.50	PHYSPROP

4-methoxybenzoic acid C8H8O3[2, 3, 32, 35, 61, 64]



Compound Data

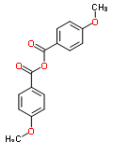
Melting point	**184.42 °C**	**457.57 K**			
CSID	10181338	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	COc1ccc(cc1)C(O)=O				
STD InChIKey	ZEYHEAKUIGZSGI-UHFFFAOYAA				

Melting Points

mp °C	source
184.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
184.00	Alfa Aesar
185.00	DrugBank
185.00	EPISuite-ChemSpider
183.50	Oxford University MSDS
185.00	PHYSPROP

4-methoxybenzoic anhydride C16H14O5[3, 64]

Compound Data



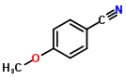
Melting point	**95.75 °C**	**368.90 K**			
CSID	63122	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	286.2794	**H bond donors**	0	**ACD/LogP**	3.35
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.22 g/cm^3
SMILES	O=C(OC(=O)c1ccc(OC)cc1)c2ccc(OC)cc2				
STD InChIKey	YGMHIBLUWGDWKP-UHFFFAOYAW				

Melting Points

mp °C	source
97.00	Alfa Aesar
94.50	PHYSPROP

4-methoxybenzonitrile C8H7NO[2, 3, 64]

Compound Data



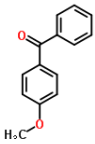
Melting point	**59.83 °C**	**332.98 K**			
CSID	21112332	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	133.1473	**H bond donors**	0	**ACD/LogP**	1.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	COc1ccc(C#N)cc1				
STD InChIKey	XDJAAZYHCCRJOK-UHFFFAOYAA				

Melting Points

mp °C	source
59.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
59.00	Alfa Aesar
61.50	PHYSPROP

4-methoxybenzophenone C14H12O2[3, 64]

Compound Data



Melting point	**61.75 °C**	**334.90 K**			
CSID	62361	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	0	**ACD/LogP**	3.23
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=C(c1ccc(OC)cc1)c2ccccc2				
STD InChIKey	SWFHGTMLYIBPPA-UHFFFAOYAU				

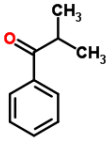
Melting Points

mp °C	source
62.00	Alfa Aesar
61.50	PHYSPROP

4-methoxybenzophenone C10H12O[3, 64]

Compound Data

Melting point	**-0.15 °C**	**273.00 K**			
CSID	62359	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	148.2017	**H bond donors**	0	**ACD/LogP**	2.54



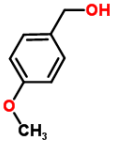
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.96 g/cm
SMILES	O=C(c1ccccc1)C(C)C				
STD InChIKey	BSMGLVDZZMBWQB-UHFFFAOYAD				

Melting Points

mp °C	source
1.00	Alfa Aesar
-1.30	PHYSPROP

4-methoxybenzyl alcohol C8H10O2[2, 3, 64]

Compound Data



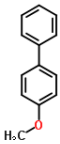
Melting point	**25.00 °C**	**298.15 K**			
CSID	21105859	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	1	**ACD/LogP**	0.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	COc1ccc(CO)cc1				
STD InChIKey	MSHFRERJPWKJFX-UHFFFAOYAE				

Melting Points

mp °C	source
26.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
24.00	Alfa Aesar
25.00	PHYSPROP

4-methoxybiphenyl C13H12O[3, 7, 64]

Compound Data



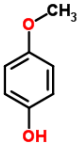
Melting point	**89.67 °C**	**362.82 K**			
CSID	11449	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.2338	**H bond donors**	0	**ACD/LogP**	3.79
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	O(c2ccc(c1ccccc1)cc2)C				
STD InChIKey	RHDYQUZYHZWTCI-UHFFFAOYAG				

Melting Points

mp °C	source
88.00	Alfa Aesar
91.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
90.00	PHYSPROP

4-methoxyphenol C7H8O2[2, 3, 61, 64, 72, 72]

Compound Data

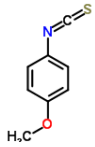


Melting point	**56.17 °C**	**329.32 K**			
CSID	8665	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	1	**ACD/LogP**	1.35
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	COc1ccc(cc1)O				
STD InChIKey	NWVVVBRKAWDGAB-UHFFFAOYAR				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
57.00	Alfa Aesar
56.00	Oxford University MSDS
57.00	PHYSPROP
55.00	Sigma-Aldrich
56.00	Sigma-Aldrich

4-methoxyphenyl isothiocyanate C8H7NOS[3, 64]



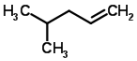
Compound Data

Melting point	**18.50 °C**	**291.65 K**			
CSID	67835	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	165.2123	**H bond donors**	0	**ACD/LogP**	3.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.08 g/cm^3
SMILES	S=C=N/c1ccc(OC)cc1				
STD InChIKey	VRPQCVLBOZOYCG-UHFFFAOYAU				

Melting Points

mp °C	source
19.00	Alfa Aesar
18.00	PHYSPROP

4-methyl-1-pentene C6H12[3, 4, 64]



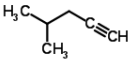
Compound Data

Melting point	**-153.53 °C**	**119.62 K**			
CSID	12201	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.68 g/cm^3
SMILES	C=C\CC(C)C				
STD InChIKey	WSSSPWUEQFSQQG-UHFFFAOYAV				

Melting Points

mp °C	source
-153.00	Alfa Aesar
-154.00	American Petroleum Institute. Research Project 44; Selected ...
-153.60	PHYSPROP

4-methyl-1-pentyne C6H10[4, 64]



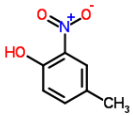
Compound Data

Melting point	**-104.80 °C**	**168.35 K**			
CSID	122546	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.73 g/cm^3
SMILES	C#CCC(C)C				
STD InChIKey	OXRWICUICBZVAE-UHFFFAOYAK				

Melting Points

mp °C	source
-105.00	American Petroleum Institute. Research Project 44; Selected ...
-104.60	PHYSPROP

4-methyl-2-nitrophenol C7H7NO3[3, 64]



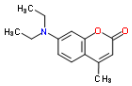
Compound Data

Melting point	**35.25 °C**	**308.40 K**			
CSID	8086	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	153.1354	**H bond donors**	1	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1O)C				
STD InChIKey	SYDNSSSQVSOXTN-UHFFFAOYAL				

Melting Points

mp °C	source
34.00	Alfa Aesar
36.50	PHYSPROP

4-methyl-7-diethylaminocoumarin C14H17NO2[3, 61]



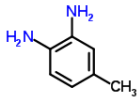
Compound Data

Melting point	**72.00 °C**	**345.15 K**			
CSID	6783	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	231.2903	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.12 g/cm^3
SMILES	O=C/2Oc1cc(ccc1\C(=C\2)C)N(CC)CC				
STD InChIKey	AFYCEAFSNDLKSX-UHFFFAOYAZ				

Melting Points

mp °C	source
74.00	Alfa Aesar
70.00	Oxford University MSDS

4-methylbenzene-1,2-diamine C7H10N2[2, 3, 61, 64]



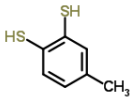
Compound Data

Melting point	**88.75 °C**	**361.90 K**			
CSID	9908	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1677	**H bond donors**	4	**ACD/LogP**	0.51
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	Nc1ccc(cc1N)C				
STD InChIKey	DGRGLKZMKWPMOH-UHFFFAOYAV				

Melting Points

mp °C	source
88.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
88.00	Alfa Aesar
89.50	Oxford University MSDS
89.50	PHYSPROP

4-methylbenzene-1,2-dithiol C7H8S2[3, 61, 64]



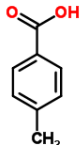
Compound Data

Melting point	**30.00 °C**	**303.15 K**			
CSID	9910	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	156.2684	**H bond donors**	0	**ACD/LogP**	3.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	Sc1ccc(cc1S)C				
STD InChIKey	NIAAGQAEVGMHPM-UHFFFAOYAZ				

Melting Points

mp °C	source
30.00	Alfa Aesar
31.00	Oxford University MSDS
29.00	PHYSPROP

4-methylbenzoic acid C8H8O2[2, 3, 35, 61, 64, 70]



Compound Data

Melting point	**180.20 °C**	**453.35 K**			
CSID	7190	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	1	**ACD/LogP**	2.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	Cc1ccc(cc1)C(=O)O				
STD InChIKey	LPNBBFKOUUSUDB-UHFFFAOYAB				

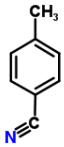
Melting Points

mp °C	source
182.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
180.00	Alfa Aesar
179.60	EPISuite-ChemSpider

180.00	Oxford University MSDS
179.60	PHYSPROP
180.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

4-methylbenzonitrile C8H7N[2, 3, 61, 64]

Compound Data



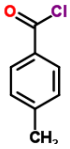
Melting point	**28.62 °C**	**301.77 K**			
CSID	21106167	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	117.1479	**H bond donors**	0	**ACD/LogP**	2.37
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.01 g/cm^3
SMILES	Cc1ccc(cc1)C#N				
STD InChIKey	VCZNNAKNUVJVGX-UHFFFAOYAI				

Melting Points

mp °C	source
28.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
28.00	Alfa Aesar
29.00	Oxford University MSDS
29.50	PHYSPROP

4-methylbenzoyl chloride C8H7ClO[3, 64]

Compound Data



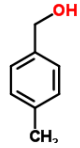
Melting point	**-2.50 °C**	**270.65 K**			
CSID	12831	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	154.5936	**H bond donors**	0	**ACD/LogP**	2.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	O=C(Cl)c1ccc(cc1)C				
STD InChIKey	NQUVCRCCRXRJCK-UHFFFAOYAS				

Melting Points

mp °C	source
-2.00	Alfa Aesar
-3.00	PHYSPROP

4-methylbenzyl alcohol C8H10O[2, 3, 64]

Compound Data



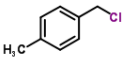
Melting point	**60.50 °C**	**333.65 K**			
CSID	11021	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	1	**ACD/LogP**	1.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.02 g/cm^3
SMILES	OCc1ccc(cc1)C				
STD InChIKey	KMTDMTZBNYGUNX-UHFFFAOYAR				

Melting Points

mp °C	source
61.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
59.00	Alfa Aesar
61.50	PHYSPROP

4-methylbenzyl chloride C8H9Cl[2, 3]

Compound Data



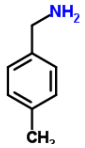
Melting point	**4.50 °C**	**277.65 K**			
CSID	21111850	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	140.6101	**H bond donors**	0	**ACD/LogP**	2.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	Cc1ccc(CCl)cc1				
STD InChIKey	DMHZDOTYAVHSEH-UHFFFAOYAF				

Melting Points

mp °C	source
4.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
5.00	Alfa Aesar

4-methylbenzylamine C8H11N[3, 64]

Compound Data



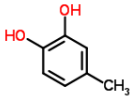
Melting point	**12.25 °C**	**285.40 K**			
CSID	59426	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	2	**ACD/LogP**	1.55
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.96 g/cm^3
SMILES	NCc1ccc(cc1)C				
STD InChIKey	HMTSWYPNXFHGEP-UHFFFAOYAJ				

Melting Points

mp °C	source
12.00	Alfa Aesar
12.50	PHYSPROP

4-methylcatechol C7H8O2[3, 64]

Compound Data



Melting point	**66.50 °C**	**339.65 K**			
CSID	9564	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	Oc1ccc(cc1O)C				
STD InChIKey	ZBCATMYQYDCTIZ-UHFFFAOYAF				

Melting Points

mp °C	source
68.00	Alfa Aesar
65.00	PHYSPROP

4-methylcyclohexanone C7H12O[3, 64]

Compound Data

Melting point	**-40.80 °C**	**232.35 K**			
CSID	11041	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	112.1696	**H bond donors**	0	**ACD/LogP**	1.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.91 g/cm^3
SMILES	O=C1CCC(C)CC1				
STD InChIKey	VGVHNLRUAMRIEW-UHFFFAOYAE				

Melting Points

mp °C	source
-41.00	Alfa Aesar
-40.60	PHYSPROP

4-methylcyclopentene C6H10[4, 64]

Compound Data

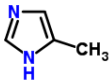
Melting point	**-160.90 °C**	**112.25 K**			
CSID	14893	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.82
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.81 g/cm^3
SMILES	C\1=C\CC(C)C/1				
STD InChIKey	FWMRUAODTCVEQK-UHFFFAOYAW				

Melting Points

mp °C	source

-161.00	American Petroleum Institute. Research Project 44; Selected ...
-160.80	PHYSPROP

4-methylimidazole C4H6N2[3, 64]



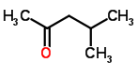
Compound Data

Melting point	**53.50 °C**	**326.65 K**					
CSID	12640	**H bond acceptors**	2	**Rule of 5 violations**	0		
Molecular weight	82.1038	**H bond donors**	1	**ACD/LogP**	0.30		
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.06 g/cm^3		
SMILES	n1cc(nc1)C						
STD InChIKey	XLSZMDLNRCVEIJ-UHFFFAOYAA						

Melting Points

mp °C	source
51.00	Alfa Aesar
56.00	PHYSPROP

4-methylpentan-2-one C6H12O[3, 4, 61, 64]



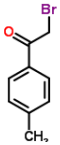
Compound Data

Melting point	**-83.00 °C**	**190.15 K**					
CSID	7621	**H bond acceptors**	1	**Rule of 5 violations**	0		
Molecular weight	100.1589	**H bond donors**	0	**ACD/LogP**	1.25		
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.80 g/cm^3		
SMILES	O=C(C)CC(C)C						
STD InChIKey	NTIZESTWPVYFNL-UHFFFAOYAQ						

Melting Points

mp °C	source
-84.00	Alfa Aesar
-84.00	American Petroleum Institute. Research Project 44; Selected ...
-80.00	Oxford University MSDS
-84.00	PHYSPROP

4-methylphenacyl bromide C9H9BrO[3, 64]



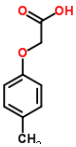
Compound Data

Melting point	**51.50 °C**	**324.65 K**					
CSID	62483	**H bond acceptors**	1	**Rule of 5 violations**	0		
Molecular weight	213.0712	**H bond donors**	0	**ACD/LogP**	2.65		
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.42 g/cm^3		
SMILES	O=C(c1ccc(cc1)C)CBr						
STD InChIKey	KRVGXFREOJHJAX-UHFFFAOYAC						

Melting Points

mp °C	source
52.00	Alfa Aesar
51.00	PHYSPROP

4-methylphenoxyacetic acid C9H10O3[3, 64]



Compound Data

Melting point	**140.50 °C**	**413.65 K**					
CSID	63512	**H bond acceptors**	3	**Rule of 5 violations**	0		
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	1.80		
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3		
SMILES	O=C(O)COc1ccc(cc1)C						
STD InChIKey	SFTDDFBJWUWKMN-UHFFFAOYAF						

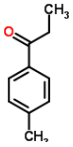
Melting Points

mp °C	source

140.00	Alfa Aesar
141.00	PHYSPROP

4-methylpropiophenone C10H12O[3, 64]

Compound Data



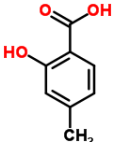
Melting point	**7.10 °C**	**280.25 K**			
CSID	20140	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	148.2017	**H bond donors**	0	**ACD/LogP**	2.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.96 g/cm^3
SMILES	O=C(c1ccc(cc1)C)CC				
STD InChIKey	PATYHUUYADUHQS-UHFFFAOYAY				

Melting Points

mp °C	source
7.00	Alfa Aesar
7.20	PHYSPROP

4-methylsalicylic acid C8H8O3[3, 64]

Compound Data



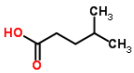
Melting point	**177.50 °C**	**450.65 K**			
CSID	5584	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.30 g/cm^3
SMILES	O=C(O)c1ccc(cc1O)C				
STD InChIKey	NJESAXZANHETJV-UHFFFAOYAQ				

Melting Points

mp °C	source
178.00	Alfa Aesar
177.00	PHYSPROP

4-methylvaleric acid C6H12O2[3, 64]

Compound Data



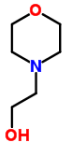
Melting point	**-34.00 °C**	**239.15 K**			
CSID	12067	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	1	**ACD/LogP**	1.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.95 g/cm^3
SMILES	O=C(O)CCC(C)C				
STD InChIKey	FGKJLKRYENPLQH-UHFFFAOYAB				

Melting Points

mp °C	source
-35.00	Alfa Aesar
-33.00	PHYSPROP

4-morpholineethanol C6H13NO2[3, 64]

Compound Data



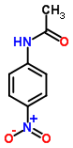
Melting point	**0.20 °C**	**273.35 K**			
CSID	55110	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	131.1729	**H bond donors**	1	**ACD/LogP**	-0.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.06 g/cm^3
SMILES	OCCN1CCOCC1				
STD InChIKey	KKFDCBRMNNSAAW-UHFFFAOYAD				

Melting Points

mp °C	source
2.00	Alfa Aesar
-1.60	PHYSPROP

4-nitroacetanilide $C_8H_8N_2O_3$[3, 61, 64]

Compound Data



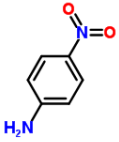
Melting point	**215.67 °C**	**488.82 K**			
CSID	7407	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	180.1607	**H bond donors**	1	**ACD/LogP**	1.66
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=C(Nc1ccc(cc1)[N+]([O-])=O)C				
STD InChIKey	NQRLPDFELNCFHW-UHFFFAOYAB				

Melting Points

mp °C	source
216.00	Alfa Aesar
215.00	Oxford University MSDS
216.00	PHYSPROP

4-nitroaniline $C_6H_6N_2O_2$[2, 3, 61, 64, 72]

Compound Data



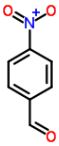
Melting point	**147.90 °C**	**421.05 K**			
CSID	13846959	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	138.124	**H bond donors**	2	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	c1cc(ccc1N)N(=O)=O				
STD InChIKey	TYMLOMAKGOJONV-UHFFFAOYAW				

Melting Points

mp °C	source
150.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
148.00	Alfa Aesar
148.00	Oxford University MSDS
146.00	PHYSPROP
147.50	Sigma-Aldrich

4-nitrobenzaldehyde $C_7H_5NO_3$[2, 3, 3, 64]

Compound Data



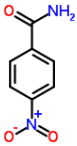
Melting point	**106.25 °C**	**379.40 K**			
CSID	526	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	151.1195	**H bond donors**	0	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C=O)cc1				
STD InChIKey	BXRFQSNOROATLV-UHFFFAOYAO				

Melting Points

mp °C	source
108.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
105.00	Alfa Aesar
105.00	Alfa Aesar
107.00	PHYSPROP

4-nitrobenzamide $C_7H_6N_2O_3$[3, 7, 61, 64]

Compound Data



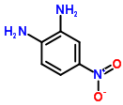
Melting point	**200.88 °C**	**474.02 K**			
CSID	11594	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	166.1341	**H bond donors**	2	**ACD/LogP**	0.82
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.38 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C(=O)N)cc1				
STD InChIKey	ZESWUEBPRPGMTP-UHFFFAOYAG				

Melting Points

mp °C	source
200.00	Alfa Aesar
201.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
202.50	Oxford University MSDS
200.00	PHYSPROP

4-nitrobenzene-1,2-diamine C6H7N3O2[3, 61, 64]

Compound Data



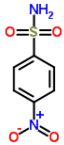
Melting point	**199.83 °C**	**472.98 K**			
CSID	4286892	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	153.1387	**H bond donors**	4	**ACD/LogP**	1.21
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.45 g/cm^3
SMILES	[O-][N+](=O)c1cc(N)c(N)cc1				
STD InChIKey	RAUWPNXIALNKQM-UHFFFAOYAF				

Melting Points

mp °C	source
201.00	Alfa Aesar
199.00	Oxford University MSDS
199.50	PHYSPROP

4-nitrobenzenesulfonamide C6H6N2O4S[3, 64]

Compound Data



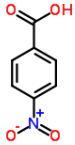
Melting point	**179.50 °C**	**452.65 K**			
CSID	21360	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	202.1878	**H bond donors**	2	**ACD/LogP**	0.65
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.55 g/cm^3
SMILES	O=S(=O)(N)c1ccc([N+]([O-])=O)cc1				
STD InChIKey	QWKKYJLAUWFPDB-UHFFFAOYAH				

Melting Points

mp °C	source
180.00	Alfa Aesar
179.00	PHYSPROP

4-nitrobenzoic acid C7H5NO4[2, 3, 35, 61, 64]

Compound Data



Melting point	**240.40 °C**	**513.55 K**			
CSID	5882	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	167.1189	**H bond donors**	1	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C(=O)O)cc1				
STD InChIKey	OTLNPYWUJOZPPA-UHFFFAOYAB				

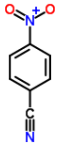
Melting Points

mp °C	source
241.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
240.00	Alfa Aesar
242.00	EPISuite-ChemSpider
237.00	Oxford University MSDS
242.00	PHYSPROP

4-nitrobenzonitrile C7H4N2O2[2, 3, 64]

Compound Data

Melting point	**147.17 °C**	**420.32 K**			
CSID	11593	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	148.1189	**H bond donors**	0	**ACD/LogP**	1.19



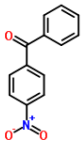
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.31 g/cm^3
SMILES	N#Cc1ccc([N+]([O-])=O)cc1				
STD InChIKey	NKJIFDNZPGLLSH-UHFFFAOYAP				

Melting Points

mp °C	source
149.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
145.00	Alfa Aesar
147.50	PHYSPROP

4-nitrobenzophenone C13H9NO3[3, 64]

Compound Data



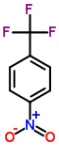
Melting point	**137.50 °C**	**410.65 K**			
CSID	64003	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	227.2155	**H bond donors**	0	**ACD/LogP**	3.05
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	O=[N+]([O-])c2ccc(C(=O)c1ccccc1)cc2				
STD InChIKey	ZYMCBJWUWHHVRX-UHFFFAOYAN				

Melting Points

mp °C	source
137.00	Alfa Aesar
138.00	PHYSPROP

4-nitrobenzotrifluoride C7H4F3NO2[3, 61, 64]

Compound Data



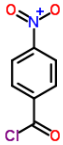
Melting point	**39.33 °C**	**312.48 K**			
CSID	9438	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	191.1074	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.42 g/cm^3
SMILES	c1cc(ccc1C(F)(F)F)[N+](=O)[O-]				
STD InChIKey	XKYLCLMYQDFGKO-UHFFFAOYAM				

Melting Points

mp °C	source
40.00	Alfa Aesar
39.00	Oxford University MSDS
39.00	PHYSPROP

4-nitrobenzoyl chloride C7H4ClNO3[3, 61, 64]

Compound Data



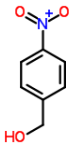
Melting point	**74.33 °C**	**347.48 K**			
CSID	8188	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	185.5646	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.45 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C(Cl)=O)cc1				
STD InChIKey	SKDHHIUENRGTHK-UHFFFAOYAC				

Melting Points

mp °C	source
73.00	Alfa Aesar
75.00	Oxford University MSDS
75.00	PHYSPROP

4-nitrobenzyl alcohol C7H7NO3[2, 3, 64]

Compound Data



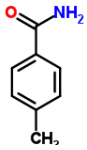
Melting point	**94.83 °C**	**367.98 K**			
CSID	62486	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	153.1354	**H bond donors**	1	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.33 g/cm^3
SMILES	[O-][N+](=O)c1ccc(cc1)CO				
STD InChIKey	JKTYGPATCNUWKN-UHFFFAOYAT				

Melting Points

mp °C	source
94.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
94.00	Alfa Aesar
96.50	PHYSPROP

4-nitrobenzyl alcohol C8H9NO[2, 3, 64]

Compound Data



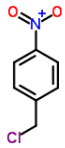
Melting point	**161.33 °C**	**434.48 K**			
CSID	62485	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	2	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	O=C(c1ccc(cc1)C)N				
STD InChIKey	UHBGYFCCKRAEHA-UHFFFAOYAA				

Melting Points

mp °C	source
163.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
159.00	Alfa Aesar
162.00	PHYSPROP

4-nitrobenzyl chloride C7H6ClNO2[2, 3, 61, 64]

Compound Data



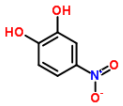
Melting point	**71.75 °C**	**344.90 K**			
CSID	7202	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.581	**H bond donors**	0	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	ClCc1ccc([N+]([O-])=O)cc1				
STD InChIKey	KGCNHWXDPDPSBV-UHFFFAOYAY				

Melting Points

mp °C	source
73.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
72.00	Alfa Aesar
71.00	Oxford University MSDS
71.00	PHYSPROP

4-nitrocatechol C6H5NO4[3, 64]

Compound Data

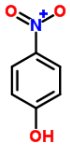


Melting point	**175.50 °C**	**448.65 K**			
CSID	2745027	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	155.1082	**H bond donors**	2	**ACD/LogP**	1.68
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.58 g/cm^3
SMILES	[O-][N+](=O)c1cc(O)c(O)cc1				
STD InChIKey	XJNPNXSISMKQEX-UHFFFAOYAU				

Melting Points

mp °C	source
176.00	Alfa Aesar
175.00	PHYSPROP

4-nitrophenol C6H5NO3[2, 3, 48, 64, 72]



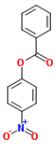
Compound Data

Melting point	**113.26 °C**	**386.41 K**			
CSID	955	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	139.1088	**H bond donors**	1	**ACD/LogP**	1.67
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.40 g/cm^3
SMILES	c1cc(ccc1[N+](=O)[O-])O				
STD InChIKey	BTJIUGUIPKRLHP-UHFFFAOYAP				

Melting Points

mp °C	source
115.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
113.00	Alfa Aesar
112.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
113.80	PHYSPROP
112.50	Sigma-Aldrich

4-nitrophenyl benzoate C13H9NO4[3, 48]



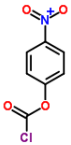
Compound Data

Melting point	**141.00 °C**	**414.15 K**			
CSID	63575	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	243.2149	**H bond donors**	0	**ACD/LogP**	3.77
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.32 g/cm^3
SMILES	O=C(Oc1ccc(cc1)[N+]([O-])=O)c2ccccc2				
STD InChIKey	GMKZBFFLCONHDE-UHFFFAOYAZ				

Melting Points

mp °C	source
143.00	Alfa Aesar
139.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

4-nitrophenyl chloroformate C7H4ClNO4[3, 61]



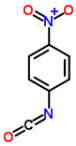
Compound Data

Melting point	**78.50 °C**	**351.65 K**			
CSID	74123	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	0	**ACD/LogP**	2.84
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.51 g/cm^3
SMILES	O=C(Cl)Oc1ccc(cc1)[N+](O-])=O				
STD InChIKey	NXLNNXIXOYSCMB-UHFFFAOYAH				

Melting Points

mp °C	source
79.00	Alfa Aesar
78.00	Oxford University MSDS

4-nitrophenyl isocyanate C7H4N2O3[3, 64]



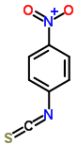
Compound Data

Melting point	**57.50 °C**	**330.65 K**			
CSID	59403	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	164.1183	**H bond donors**	0	**ACD/LogP**	2.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=C=N\c1ccc(cc1)[N+](O-])=O				
STD InChIKey	GFNKTLQTQSALEJ-UHFFFAOYAM				

Melting Points

mp °C	source
58.00	Alfa Aesar
57.00	PHYSPROP

4-nitrophenyl isothiocyanate C7H4N2O2S[3, 64]



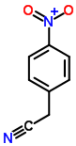
Compound Data

Melting point	**109.50 °C**	**382.65 K**			
CSID	67597	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	180.1839	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	S=C=N\c1ccc(cc1)[N+]([O-])=O				
STD InChIKey	NXHSSIGRWJENBH-UHFFFAOYAJ				

Melting Points

mp °C	source
108.00	Alfa Aesar
111.00	PHYSPROP

4-nitrophenylacetonitrile C8H6N2O2[2, 3, 48, 64]



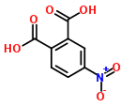
Compound Data

Melting point	**116.25 °C**	**389.40 K**			
CSID	61672	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	162.1454	**H bond donors**	0	**ACD/LogP**	1.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	N#CCc1ccc(cc1)[N+]([O-])=O				
STD InChIKey	PXNJGLAVKOXITN-UHFFFAOYAC				

Melting Points

mp °C	source
116.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
116.00	Alfa Aesar
116.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
117.00	PHYSPROP

4-nitrophthalic acid C8H5NO6[3, 48]



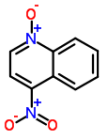
Compound Data

Melting point	**162.50 °C**	**435.65 K**			
CSID	62338	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	211.1284	**H bond donors**	2	**ACD/LogP**	1.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.67 g/cm^3
SMILES	O=[N+]([O-])c1cc(c(C(=O)O)cc1)C(=O)O				
STD InChIKey	SLBQXWXKPNIVSQ-UHFFFAOYAK				

Melting Points

mp °C	source
163.00	Alfa Aesar
162.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

4-nitroquinoline N-oxide C9H6N2O3[3, 61, 64]



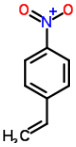
Compound Data

Melting point	**154.33 °C**	**427.48 K**			
CSID	5740	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	190.1555	**H bond donors**	0	**ACD/LogP**	0.92
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.42 g/cm^3
SMILES	[O-][N+](=O)c2c1c(cccc1)[n+]([O-])cc2				
STD InChIKey	YHQDZJICGQWFHK-UHFFFAOYAP				

Melting Points

mp °C	source
155.00	Alfa Aesar
154.00	Oxford University MSDS
154.00	PHYSPROP

4-nitrostyrene $C_8H_7NO_2$[3, 7]



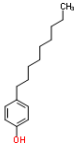
Compound Data

Melting point	**28.00 °C**	**301.15 K**			
CSID	7201	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	149.1467	**H bond donors**	0	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=[N+]([O-])c1ccc(\C=C)cc1				
STD InChIKey	YFZHODLXYNDBSM-UHFFFAOYAA				

Melting Points

mp °C	source
27.00	Alfa Aesar
29.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-nonylphenol $C_{15}H_{24}O$[3, 64]



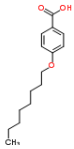
Compound Data

Melting point	**43.50 °C**	**316.65 K**			
CSID	1688	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	220.3505	**H bond donors**	1	**ACD/LogP**	6.19
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	0.93 g/cm^3
SMILES	Oc1ccc(cc1)CCCCCCCCC				
STD InChIKey	IGFHQQFPSIBGKE-UHFFFAOYAO				

Melting Points

mp °C	source
45.00	Alfa Aesar
42.00	PHYSPROP

4-octyloxybenzoic acid $C_{15}H_{22}O_3$[3, 48]



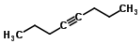
Compound Data

Melting point	**102.00 °C**	**375.15 K**			
CSID	16310	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	250.3334	**H bond donors**	1	**ACD/LogP**	5.68
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.04 g/cm^3
SMILES	O=C(O)c1ccc(OCCCCCCCC)cc1				
STD InChIKey	IALWCYFULVHLEC-UHFFFAOYAX				

Melting Points

mp °C	source
103.00	Alfa Aesar
101.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

4-octyne C_8H_{14}[2, 64]



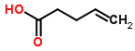
Compound Data

Melting point	**-102.00 °C**	**171.15 K**			
CSID	15221	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	3.51
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.77 g/cm^3
SMILES	CCCC#CCCC				
STD InChIKey	GZTNBKQTTZSQNS-UHFFFAOYAB				

Melting Points

mp °C	source
-103.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-101.00	PHYSPROP

4-pentenoic acid $C_5H_8O_2$[3, 64]



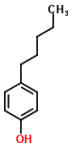
Compound Data

Melting point	**-22.25 °C**	**250.90 K**			
CSID	55085	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1158	**H bond donors**	1	**ACD/LogP**	0.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.99 g/cm^3
SMILES	O=C(O)CC\C=C				
STD InChIKey	HVAMZGADVCBITI-UHFFFAOYAW				

Melting Points

mp °C	source
-22.00	Alfa Aesar
-22.50	PHYSPROP

4-pentylphenol C11H16O[3, 64]



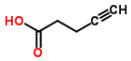
Compound Data

Melting point	**23.50 °C**	**296.65 K**			
CSID	25119	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	164.2441	**H bond donors**	1	**ACD/LogP**	4.07
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.96 g/cm^3
SMILES	Oc1ccc(cc1)CCCCC				
STD InChIKey	ZNPSUQQXTRRSBM-UHFFFAOYAD				

Melting Points

mp °C	source
24.00	Alfa Aesar
23.00	PHYSPROP

4-pentynoic acid C5H6O2[3, 64]



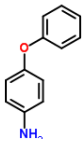
Compound Data

Melting point	**56.85 °C**	**330.00 K**			
CSID	21069	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	98.0999	**H bond donors**	1	**ACD/LogP**	0.43
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.10 g/cm^3
SMILES	O=C(O)CCC#C				
STD InChIKey	MLBYLEUJXUBIJJ-UHFFFAOYAV				

Melting Points

mp °C	source
56.00	Alfa Aesar
57.70	PHYSPROP

4-phenoxyaniline C12H11NO[3, 64]



Compound Data

Melting point	**83.50 °C**	**356.65 K**			
CSID	8434	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	185.2218	**H bond donors**	2	**ACD/LogP**	2.36
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	O(c1ccccc1)c2ccc(cc2)N				
STD InChIKey	WOYZXEVUWXQVNV-UHFFFAOYAE				

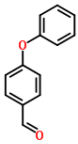
Melting Points

mp °C	source
84.00	Alfa Aesar
83.00	PHYSPROP

4-phenoxybenzaldehyde C13H10O2[3, 64]

Compound Data

Melting point	**24.75 °C**	**297.90 K**



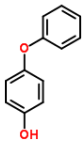
CSID	59526	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2173	**H bond donors**	0	**ACD/LogP**	3.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	O=Cc2ccc(Oc1ccccc1)cc2				
STD InChIKey	QWLHJVDRPZNVBS-UHFFFAOYAO				

Melting Points

mp °C	source
25.00	Alfa Aesar
24.50	PHYSPROP

4-phenoxyphenol C12H10O2[3, 61, 64]

Compound Data



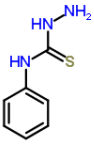
Melting point	**82.67 °C**	**355.82 K**			
CSID	12696	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	1	**ACD/LogP**	3.35
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3
SMILES	O(c1ccccc1)c2ccc(O)cc2				
STD InChIKey	ZSBDGXGICLIJGD-UHFFFAOYAU				

Melting Points

mp °C	source
84.00	Alfa Aesar
80.00	Oxford University MSDS
84.00	PHYSPROP

4-phenyl-3-thiosemicarbazide C7H9N3S[3, 64]

Compound Data



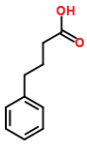
Melting point	**138.50 °C**	**411.65 K**			
CSID	638258	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	167.2315	**H bond donors**	4	**ACD/LogP**	0.93
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	S=C(Nc1ccccc1)NN				
STD InChIKey	KKIGUVBJOHCXSP-UHFFFAOYAT				

Melting Points

mp °C	source
138.00	Alfa Aesar
139.00	PHYSPROP

4-phenylbutyric acid C10H12O2[3, 35, 48, 64]

Compound Data

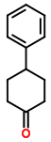


Melting point	**50.75 °C**	**323.90 K**			
CSID	4611	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	1	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	O=C(O)CCCc1ccccc1				
STD InChIKey	OBKXEAXTFZPCHS-UHFFFAOYAV				

Melting Points

mp °C	source
51.00	Alfa Aesar
52.00	EPISuite-ChemSpider
48.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
52.00	PHYSPROP

4-phenylcyclohexanone C12H14O[3, 64]



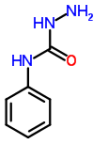
Compound Data

Melting point	**79.75 °C**	**352.90 K**			
CSID	70962	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	174.239	**H bond donors**	0	**ACD/LogP**	2.45
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	O=C2CCC(c1ccccc1)CC2				
STD InChIKey	YKAYMASDSHFOGI-UHFFFAOYAM				

Melting Points

mp °C	source
80.00	Alfa Aesar
79.50	PHYSPROP

4-phenylsemicarbazide C7H9N3O[3, 64]



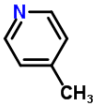
Compound Data

Melting point	**126.00 °C**	**399.15 K**			
CSID	10380	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	151.1659	**H bond donors**	4	**ACD/LogP**	0.13
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	O=C(Nc1ccccc1)NN				
STD InChIKey	MOCKWYUCPREFCZ-UHFFFAOYAJ				

Melting Points

mp °C	source
124.00	Alfa Aesar
128.00	PHYSPROP

4-picoline C6H7N[3, 64]



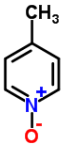
Compound Data

Melting point	**3.33 °C**	**276.48 K**			
CSID	13874733	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	93.1265	**H bond donors**	0	**ACD/LogP**	1.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.94 g/cm^3
SMILES	Cc1ccncc1				
STD InChIKey	FKNQCJSGGFJEIZ-UHFFFAOYAZ				

Melting Points

mp °C	source
3.00	Alfa Aesar
3.66	PHYSPROP

4-picoline N-oxide C6H7NO[3, 11, 17, 64]



Compound Data

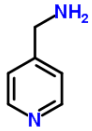
Melting point	**184.50 °C**	**457.65 K**			
CSID	13257	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	0	**ACD/LogP**	-0.74
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.01 g/cm^3
SMILES	[O-][n+]1ccc(cc1)C				
STD InChIKey	IWYYIZOHWPCALJ-UHFFFAOYAY				

Melting Points

mp °C	source
184.00	Alfa Aesar
185.50	Boekelheide V; Linn WJ. Journal of the American Chemical Soc...
184.00	ChemBlink
	Values not used in calculating the average melting point
39.00	PHYSPROP[1]

1. clearly out of range JCB

4-picolinylamine C6H8N2[3, 64]



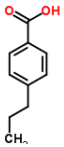
Compound Data

Melting point	**-7.80 °C**	**265.35 K**			
CSID	69736	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	2	**ACD/LogP**	-0.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	n1ccc(cc1)CN				
STD InChIKey	TXQWFIVRZNOPCK-UHFFFAOYAD				

Melting Points

mp °C	source
-8.00	Alfa Aesar
-7.60	PHYSPROP

4-propylbenzoic acid C10H12O2[3, 64]



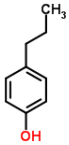
Compound Data

Melting point	**142.50 °C**	**415.65 K**			
CSID	121262	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	1	**ACD/LogP**	3.42
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	O=C(O)c1ccc(cc1)CCC				
STD InChIKey	ATZHGRNFEFVDDJ-UHFFFAOYAC				

Melting Points

mp °C	source
142.00	Alfa Aesar
143.00	PHYSPROP

4-propylphenol C9H12O[3, 31, 64]



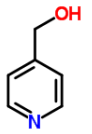
Compound Data

Melting point	**21.67 °C**	**294.82 K**			
CSID	12060	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	1	**ACD/LogP**	3.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.99 g/cm^3
SMILES	Oc1ccc(cc1)CCC				
STD InChIKey	KLSLBUSXWBJMEC-UHFFFAOYAR				

Melting Points

mp °C	source
21.00	Alfa Aesar
22.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
22.00	PHYSPROP

4-pyridinemethanol C6H7NO[3, 64]



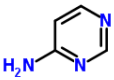
Compound Data

Melting point	**53.50 °C**	**326.65 K**			
CSID	10988	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	1	**ACD/LogP**	-0.46
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.13 g/cm^3
SMILES	OCc1ccncc1				
STD InChIKey	PTMBWNZJOQBTBK-UHFFFAOYAW				

Melting Points

mp °C	source
54.00	Alfa Aesar
53.00	PHYSPROP

4-pyrimidinamine C4H5N3[3, 64]



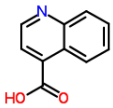
Compound Data

Melting point	**152.50 °C**	**425.65 K**			
CSID	62181	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	95.1026	**H bond donors**	2	**ACD/LogP**	-0.25
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.22 g/cm^3
SMILES	n1ccc(nc1)N				
STD InChIKey	OYRRZWATULMEPF-UHFFFAOYAG				

Melting Points

mp °C	source
150.00	Alfa Aesar
155.00	PHYSPROP

4-quinolinecarboxylic acid C10H7NO2[3, 64]



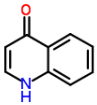
Compound Data

Melting point	**254.25 °C**	**527.40 K**			
CSID	9826	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	173.1681	**H bond donors**	1	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	O=C(O)c1c2ccccc2ncc1				
STD InChIKey	VQMSRUREDGBWKT-UHFFFAOYAV				

Melting Points

mp °C	source
254.00	Alfa Aesar
254.50	PHYSPROP

4-quinolone C9H7NO[3, 64]



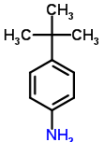
Compound Data

Melting point	**202.00 °C**	**475.15 K**			
CSID	62357	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	145.158	**H bond donors**	1	**ACD/LogP**	2.50
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	O=C\2c1c(cccc1)N/C=C/2				
STD InChIKey	PMZDQRJGMBOQBF-UHFFFAOYAZ				

Melting Points

mp °C	source
203.00	Alfa Aesar
201.00	PHYSPROP

4-t-butylaniline C10H15N[2, 3, 64]



Compound Data

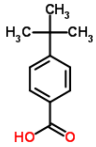
Melting point	**16.00 °C**	**289.15 K**			
CSID	63057	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	149.2328	**H bond donors**	2	**ACD/LogP**	2.62
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.94 g/cm^3
SMILES	Nc1ccc(cc1)C(C)(C)C				
STD InChIKey	WRDWWAVNELMWAM-UHFFFAOYAC				

Melting Points

mp °C	source
15.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
16.00	Alfa Aesar
17.00	PHYSPROP

4-t-butylbenzoic acid C11H14O2[2, 3, 64]

Compound Data



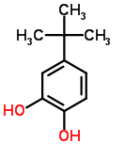
Melting point	**165.17 °C**	**438.32 K**			
CSID	7125	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	178.2277	**H bond donors**	1	**ACD/LogP**	3.58
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	O=C(O)c1ccc(cc1)C(C)(C)C				
STD InChIKey	KDVYCTOWXSLNNI-UHFFFAOYAA				

Melting Points

mp °C	source
165.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
166.00	Alfa Aesar
164.50	PHYSPROP

4-t-butylcatechol C10H14O2[3, 64]

Compound Data



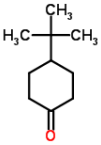
Melting point	**54.65 °C**	**327.80 K**			
CSID	7103	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	166.217	**H bond donors**	2	**ACD/LogP**	2.57
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.09 g/cm^3
SMILES	Oc1ccc(cc1O)C(C)(C)C				
STD InChIKey	XESZUVZBAMCAEJ-UHFFFAOYAR				

Melting Points

mp °C	source
55.00	Alfa Aesar
54.30	PHYSPROP

4-t-butylcyclohexanone C10H18O[2, 3, 64]

Compound Data



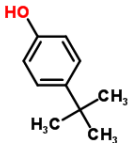
Melting point	**48.83 °C**	**321.98 K**			
CSID	7114	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	154.2493	**H bond donors**	0	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.91 g/cm^3
SMILES	O=C1CCC(C(C)(C)C)CC1				
STD InChIKey	YKFKEYKJGVSEIX-UHFFFAOYAP				

Melting Points

mp °C	source
49.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
49.00	Alfa Aesar
48.50	PHYSPROP

4-t-butylphenol C10H14O[3, 31, 64, 72]

Compound Data

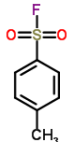


Melting point	**98.88 °C**	**372.02 K**			
CSID	13846663	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	1	**ACD/LogP**	3.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	CC(C)(C)c1ccc(cc1)O				
STD InChIKey	QHPQWRBYOIRBIT-UHFFFAOYAM				

Melting Points

mp °C	source
99.00	Alfa Aesar
100.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
98.00	PHYSPROP
98.50	Sigma-Aldrich

4-toluenesulfonyl fluoride C7H7FO2S[3, 64]



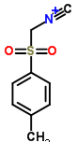
Compound Data

Melting point	**41.25 °C**	**314.40 K**			
CSID	9571	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	174.1927	**H bond donors**	0	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.28 g/cm^3
SMILES	O=S(F)(=O)c1ccc(cc1)C				
STD InChIKey	IZZYABADQVQHLC-UHFFFAOYAQ				

Melting Points

mp °C	source
41.00	Alfa Aesar
41.50	PHYSPROP

4-toluenesulfonylmethyl isocyanide C9H9NO2S[3, 3]



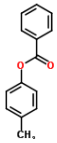
Compound Data

Melting point	**112.25 °C**	**385.40 K**			
CSID	142204	**H bond acceptors**	3	**Rule of 5 violations**	NA
Molecular weight	195.2383	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.00 g/cm^3
SMILES	O=S(=O)(c1ccc(cc1)C)C[N+]#[C-]				
STD InChIKey	CFOAUYCPAUGDFF-UHFFFAOYAC				

Melting Points

mp °C	source
112.50	Alfa Aesar
112.00	Alfa Aesar

4-tolyl benzoate C14H12O2[7, 48, 64]



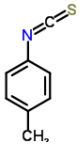
Compound Data

Melting point	**70.50 °C**	**343.65 K**			
CSID	11468	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	0	**ACD/LogP**	4.05
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.12 g/cm^3
SMILES	O=C(Oc1ccc(cc1)C)c2ccccc2				
STD InChIKey	LLRZUDIHEZXFGV-UHFFFAOYAP				

Melting Points

mp °C	source
70.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
70.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
71.50	PHYSPROP

4-tolyl isothiocyanate C8H7NS[3, 64]



Compound Data

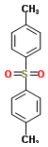
Melting point	**25.25 °C**	**298.40 K**			
CSID	11650	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	149.2129	**H bond donors**	0	**ACD/LogP**	3.70
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.02 g/cm^3
SMILES	S=C=N\c1ccc(cc1)C				
STD InChIKey	ABQKHKWXTUVKGF-UHFFFAOYAX				

Melting Points

mp °C	source
25.00	Alfa Aesar
25.50	PHYSPROP

4-tolyl sulfone C14H14O2S[3, 64]

Compound Data



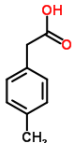
Melting point	**158.00 °C**	**431.15 K**			
CSID	62252	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	246.3248	**H bond donors**	0	**ACD/LogP**	3.32
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=S(=O)(c1ccc(cc1)C)c2ccc(cc2)C				
STD InChIKey	WEAYCYAIVOIUMG-UHFFFAOYAO				

Melting Points

mp °C	source
157.00	Alfa Aesar
159.00	PHYSPROP

4-tolylacetic acid C9H10O2[3, 64]

Compound Data



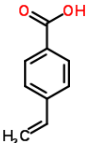
Melting point	**92.50 °C**	**365.65 K**			
CSID	217532	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	1	**ACD/LogP**	1.97
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.13 g/cm^3
SMILES	O=C(O)Cc1ccc(cc1)C				
STD InChIKey	GXXXUZIRGXYDFP-UHFFFAOYAI				

Melting Points

mp °C	source
92.00	Alfa Aesar
93.00	PHYSPROP

4-vinylbenzoic acid C9H8O2[2, 3, 64]

Compound Data



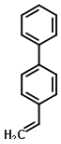
Melting point	**142.50 °C**	**415.65 K**			
CSID	13476	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	148.1586	**H bond donors**	1	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.16 g/cm^3
SMILES	O=C(O)c1ccc(\C=C)cc1				
STD InChIKey	IRQWEODKXLDORP-UHFFFAOYAQ				

Melting Points

mp °C	source
142.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
142.00	Alfa Aesar
143.50	PHYSPROP

4-vinylbiphenyl C14H12[3, 7]

Compound Data



Melting point	**117.50 °C**	**390.65 K**			
CSID	15998	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	180.2451	**H bond donors**	0	**ACD/LogP**	4.46
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.00 g/cm^3
SMILES	c1cc(ccc1)c2ccc(cc2)\C=C				
STD InChIKey	HDBWAWNLGGMZRQ-UHFFFAOYAS				

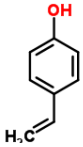
Melting Points

mp °C	source
116.00	Alfa Aesar
119.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

4-vinylphenol C8H8O[7, 64]

Compound Data

Melting point	**73.25 °C**	**346.40 K**

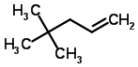


CSID	56234	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	120.1485	**H bond donors**	1	**ACD/LogP**	2.16
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	Oc1ccc(\C=C)cc1				
STD InChIKey	FUGYGGDSWSUORM-UHFFFAOYAQ				

Melting Points

mp °C	source
73.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
73.50	PHYSPROP

4,4-dimethyl-1-pentene C7H14[4, 64]



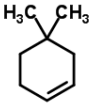
Compound Data

Melting point	**-136.80 °C**	**136.35 K**			
CSID	12444	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.70 g/cm^3
SMILES	C=C\CC(C)(C)C				
STD InChIKey	KLCNJIQZXOQYTE-UHFFFAOYAT				

Melting Points

mp °C	source
-137.00	American Petroleum Institute. Research Project 44; Selected ...
-136.60	PHYSPROP

4,4-dimethylcyclohexene C8H14[4, 64]



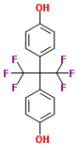
Compound Data

Melting point	**-74.20 °C**	**198.95 K**			
CSID	24634	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	3.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.80 g/cm^3
SMILES	C\1=C\CCC(C)(C)C/1				
STD InChIKey	DRORSPJLYCDESA-UHFFFAOYAG				

Melting Points

mp °C	source
-74.00	American Petroleum Institute. Research Project 44; Selected ...
-74.40	PHYSPROP

4,4'-(hexafluoroisopropylidene)diphenol C15H10F6O2[3, 64]



Compound Data

Melting point	**161.00 °C**	**434.15 K**			
CSID	66498	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	336.2291	**H bond donors**	2	**ACD/LogP**	2.82
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.45 g/cm^3
SMILES	FC(F)(F)C(c1ccc(O)cc1)(c2ccc(O)cc2)C(F)(F)F				
STD InChIKey	ZFVMWEVVKGLCIJ-UHFFFAOYAS				

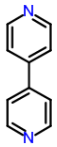
Melting Points

mp °C	source
160.00	Alfa Aesar
162.00	PHYSPROP

4,4'-bipyridine C10H8N2[3, 64]

Compound Data

Melting point	**112.00 °C**	**385.15 K**			
CSID	21105699	**H bond acceptors**	2	**Rule of 5 violations**	0



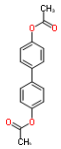
Molecular weight	156.1839	**H bond donors**	0	**ACD/LogP**	1.23
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.11 g/cm^3
SMILES	c1cnccc1c2ccncc2				
STD InChIKey	MWVTWFVJZLCBMC-UHFFFAOYAB				

Melting Points

mp °C	source
113.00	Alfa Aesar
111.00	PHYSPROP

4,4'-diacetoxybiphenyl C16H14O4[3, 48]

Compound Data



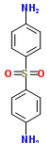
Melting point	**162.50 °C**	**435.65 K**			
CSID	525308	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	270.28	**H bond donors**	0	**ACD/LogP**	3.15
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.18 g/cm^3
SMILES	O=C(Oc1ccc(cc1)c2ccc(OC(=O)C)cc2)C				
STD InChIKey	RQMBBMQDXFZFCC-UHFFFAOYAJ				

Melting Points

mp °C	source
164.00	Alfa Aesar
161.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

4,4'-diaminodiphenyl sulfone C12H12N2O2S[3, 32, 44, 64]

Compound Data



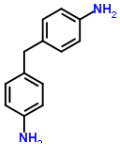
Melting point	**175.88 °C**	**449.02 K**			
CSID	2849	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	248.3009	**H bond donors**	4	**ACD/LogP**	0.94
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.36 g/cm^3
SMILES	O=S(=O)(c1ccc(N)cc1)c2ccc(N)cc2				
STD InChIKey	MQJKPEGWNLWLTK-UHFFFAOYAJ				

Melting Points

mp °C	source
177.00	Alfa Aesar
175.50	DrugBank
175.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
175.50	PHYSPROP

4,4'-diaminodiphenylmethane C13H14N2[3, 64]

Compound Data



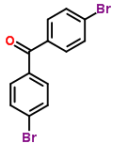
Melting point	**91.25 °C**	**364.40 K**			
CSID	7296	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2637	**H bond donors**	4	**ACD/LogP**	1.64
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.14 g/cm^3
SMILES	c1(ccc(N)cc1)Cc2ccc(N)cc2				
STD InChIKey	YBRVSVVVWCFQMG-UHFFFAOYAE				

Melting Points

mp °C	source
90.00	Alfa Aesar
92.50	PHYSPROP

4,4'-dibromobenzophenone C13H8Br2O[3, 7, 64]

Compound Data



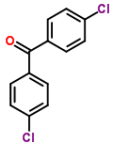
Melting point	**175.33 °C**	**448.48 K**			
CSID	65700	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	340.01	**H bond donors**	0	**ACD/LogP**	5.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.70 g/cm^3
SMILES	O=C(c1ccc(Br)cc1)c2ccc(Br)cc2				
STD InChIKey	LFABNOYDEODDFX-UHFFFAOYAS				

Melting Points

mp °C	source
174.00	Alfa Aesar
175.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
177.00	PHYSPROP

4,4'-dichlorobenzophenone C13H8Cl2O[3, 64]

Compound Data



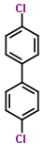
Melting point	**146.25 °C**	**419.40 K**			
CSID	6767	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	251.108	**H bond donors**	0	**ACD/LogP**	4.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=C(c1ccc(Cl)cc1)c2ccc(Cl)cc2				
STD InChIKey	OKISUZLXOYGIFP-UHFFFAOYAC				

Melting Points

mp °C	source
145.00	Alfa Aesar
147.50	PHYSPROP

4,4'-dichlorobiphenyl C12H8Cl2[64, 70]

Compound Data



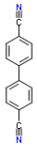
Melting point	**149.15 °C**	**422.30 K**			
CSID	15474	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	223.0979	**H bond donors**	0	**ACD/LogP**	5.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	Clc2ccc(c1ccc(Cl)cc1)cc2				
STD InChIKey	YTBRNEUEFCNVHC-UHFFFAOYAH				

Melting Points

mp °C	source
149.30	PHYSPROP
149.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

4,4'-dicyanobiphenyl C14H8N2[3, 7, 64]

Compound Data



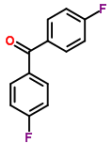
Melting point	**236.33 °C**	**509.48 K**			
CSID	14584	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	204.2267	**H bond donors**	0	**ACD/LogP**	2.94
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.20 g/cm^3
SMILES	c1cc(ccc1C#N)c2ccc(cc2)C#N				
STD InChIKey	KAXYYLCSSXFXKR-UHFFFAOYAJ				

Melting Points

mp °C	source
234.00	Alfa Aesar
237.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
238.00	PHYSPROP

4,4'-difluorobenzophenone C13H8F2O[3, 64]

Compound Data



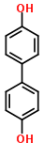
Melting point	**105.75 °C**	**378.90 K**			
CSID	9206	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	218.1988	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	O=C(c1ccc(F)cc1)c2ccc(F)cc2				
STD InChIKey	LSQARZALBDFYQZ-UHFFFAOYAZ				

Melting Points

mp °C	source
108.00	Alfa Aesar
103.50	PHYSPROP

4,4'-dihydroxybiphenyl C12H10O2[2, 3, 64]

Compound Data



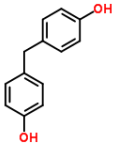
Melting point	**281.00 °C**	**554.15 K**			
CSID	6845	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2066	**H bond donors**	2	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	Oc2ccc(c1ccc(O)cc1)cc2				
STD InChIKey	VCCBEIPGXKNHFW-UHFFFAOYAM				

Melting Points

mp °C	source
278.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
282.00	Alfa Aesar
283.00	PHYSPROP

4,4'-dihydroxydiphenylmethane C13H12O2[3, 64]

Compound Data



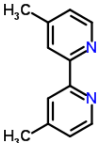
Melting point	**161.75 °C**	**434.90 K**			
CSID	11614	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	200.2332	**H bond donors**	2	**ACD/LogP**	2.73
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.21 g/cm^3
SMILES	Oc1ccc(cc1)Cc2ccc(O)cc2				
STD InChIKey	PXKLMJQFEQBVLD-UHFFFAOYAW				

Melting Points

mp °C	source
161.00	Alfa Aesar
162.50	PHYSPROP

4,4'-dimethyl-2,2'-bipyridine C12H12N2[3, 64]

Compound Data



Melting point	**174.50 °C**	**447.65 K**			
CSID	13699	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	184.2371	**H bond donors**	0	**ACD/LogP**	2.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.06 g/cm^3
SMILES	Cc1ccnc(c1)c2cc(ccn2)C				
STD InChIKey	NBPGPQJFYXNFKN-UHFFFAOYAL				

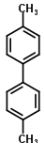
Melting Points

mp °C	source
174.00	Alfa Aesar
175.00	PHYSPROP

4,4'-dimethylbiphenyl C14H14[3, 4]

Compound Data

Melting point	**120.50 °C**	**393.65 K**



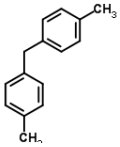
CSID	11447	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	182.261	**H bond donors**	0	**ACD/LogP**	4.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	c2c(c1ccc(cc1)C)ccc(c2)C				
STD InChIKey	RZTDESRVPFKCBH-UHFFFAOYAT				

Melting Points

mp °C	source
120.00	Alfa Aesar
121.00	American Petroleum Institute. Research Project 44; Selected ...

4,4'-dimethyldiphenylmethane C15H16[4, 64]

Compound Data



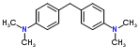
Melting point	**28.50 °C**	**301.65 K**			
CSID	19816	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	196.2875	**H bond donors**	0	**ACD/LogP**	5.13
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	c1c(ccc(c1)C)Cc2ccc(cc2)C				
STD InChIKey	HZAWPPRBCALFRN-UHFFFAOYAV				

Melting Points

mp °C	source
29.00	American Petroleum Institute. Research Project 44; Selected ...
28.00	PHYSPROP

4,4'-methylenebis(N,N-dimethylaniline) C17H22N2[3, 64]

Compound Data



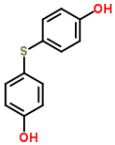
Melting point	**89.25 °C**	**362.40 K**			
CSID	21106506	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	254.37	**H bond donors**	0	**ACD/LogP**	4.42
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.04 g/cm^3
SMILES	CN(C)c2ccc(Cc1ccc(cc1)N(C)C)cc2				
STD InChIKey	JNRLEMMIVRBKJE-UHFFFAOYAR				

Melting Points

mp °C	source
87.00	Alfa Aesar
91.50	PHYSPROP

4,4'-thiodiphenol C12H10O2S[3, 64]

Compound Data



Melting point	**154.00 °C**	**427.15 K**			
CSID	16612	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	218.2716	**H bond donors**	2	**ACD/LogP**	3.34
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.37 g/cm^3
SMILES	S(c1ccc(O)cc1)c2ccc(O)cc2				
STD InChIKey	VWGKEVWFBOUAND-UHFFFAOYAP				

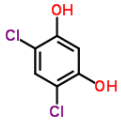
Melting Points

mp °C	source
153.00	Alfa Aesar
155.00	PHYSPROP

4,6-dichlororesorcinol C6H4Cl2O2[3, 64]

Compound Data

Melting point	**114.00 °C**	**387.15 K**			
CSID	60631	**H bond acceptors**	2	**Rule of 5 violations**	0



Molecular weight	179.0008	**H bond donors**	2	**ACD/LogP**	2.58
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.62 g/cm^3
SMILES	Clc1cc(Cl)c(O)cc1O				
STD InChIKey	GRLQBYQELUWBIO-UHFFFAOYAC				

Melting Points

mp °C	source
115.00	Alfa Aesar
113.00	PHYSPROP

5-amino-1-pentanol C5H13NO[2, 3, 64]

Compound Data

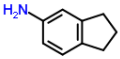
Melting point	**36.50 °C**	**309.65 K**			
CSID	68156	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	103.1628	**H bond donors**	3	**ACD/LogP**	-0.55
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	0.92 g/cm^3
SMILES	OCCCCCN				
STD InChIKey	LQGKDMHENBFVRC-UHFFFAOYAH				

Melting Points

mp °C	source
35.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
36.00	Alfa Aesar
38.50	PHYSPROP

5-aminoindane C9H11N[3, 64]

Compound Data



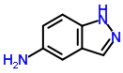
Melting point	**36.25 °C**	**309.40 K**			
CSID	81705	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	133.1903	**H bond donors**	2	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.10 g/cm^3
SMILES	c1cc(cc2c1CCC2)N				
STD InChIKey	LEWZOBYWGWKNCK-UHFFFAOYAR				

Melting Points

mp °C	source
35.00	Alfa Aesar
37.50	PHYSPROP

5-aminoindazole C7H7N3[3, 64]

Compound Data



Melting point	**175.75 °C**	**448.90 K**			
CSID	79400	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	133.1506	**H bond donors**	3	**ACD/LogP**	0.65
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	n2cc1cc(ccc1n2)N				
STD InChIKey	XBTOSRUBOXQWBO-UHFFFAOYAK				

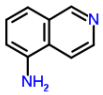
Melting Points

mp °C	source
175.00	Alfa Aesar
176.50	PHYSPROP

5-aminoisoquinoline C9H8N2[3, 64]

Compound Data

Melting point	**128.50 °C**	**401.65 K**



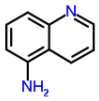
CSID	63931	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.1732	**H bond donors**	2	**ACD/LogP**	0.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	n2ccc1c(cccc1N)c2				
STD InChIKey	DTVYNUOOZIKEEX-UHFFFAOYAV				

Melting Points

mp °C	source
129.00	Alfa Aesar
128.00	PHYSPROP

5-aminoquinoline C9H8N2[3, 64]

Compound Data



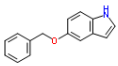
Melting point	**109.00 °C**	**382.15 K**			
CSID	11417	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.1732	**H bond donors**	2	**ACD/LogP**	0.92
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	n1cccc2c(cccc12)N				
STD InChIKey	XMIAFAKRAAMSGX-UHFFFAOYAV				

Melting Points

mp °C	source
108.00	Alfa Aesar
110.00	PHYSPROP

5-benzyloxyindole C15H13NO[3, 64]

Compound Data



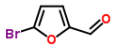
Melting point	**100.50 °C**	**373.65 K**			
CSID	13959	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	223.2698	**H bond donors**	1	**ACD/LogP**	3.71
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.20 g/cm^3
SMILES	O(c1cc2c(cc1)ncc2)Cc3ccccc3				
STD InChIKey	JCQLPDZCNSVBMS-UHFFFAOYAN				

Melting Points

mp °C	source
99.00	Alfa Aesar
102.00	PHYSPROP

5-bromo-2-furaldehyde C5H3BrO2[3, 64]

Compound Data



Melting point	**83.75 °C**	**356.90 K**			
CSID	521915	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	174.9801	**H bond donors**	0	**ACD/LogP**	1.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.75 g/cm^3
SMILES	c1cc(oc1C=O)Br				
STD InChIKey	WJTFHWXMITZNHS-UHFFFAOYAM				

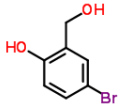
Melting Points

mp °C	source
84.00	Alfa Aesar
83.50	PHYSPROP

5-bromo-2-hydroxybenzyl alcohol C7H7BrO2[3, 64]

Compound Data

Melting point	**111.00 °C**	**384.15 K**			
CSID	67879	**H bond acceptors**	2	**Rule of 5 violations**	0



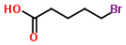
Molecular weight	203.0333	**H bond donors**	2	**ACD/LogP**	1.31
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.72 g/cm^3
SMILES	Brc1cc(c(O)cc1)CO				
STD InChIKey	KNKRHSVKIORZQB-UHFFFAOYAQ				

Melting Points

mp °C	source
109.00	Alfa Aesar
113.00	PHYSPROP

5-bromovaleric acid C5H9BrO2[3, 64]

Compound Data



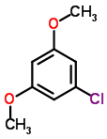
Melting point	**39.50 °C**	**312.65 K**			
CSID	15526	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	181.0278	**H bond donors**	1	**ACD/LogP**	1.38
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.52 g/cm^3
SMILES	BrCCCCC(=O)O				
STD InChIKey	WNXNUPJZWYOKMW-UHFFFAOYAD				

Melting Points

mp °C	source
40.00	Alfa Aesar
39.00	PHYSPROP

5-chloro-1,3-dimethoxybenzene C8H9ClO2[2, 3, 64]

Compound Data



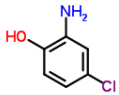
Melting point	**34.33 °C**	**307.48 K**			
CSID	73537	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.6089	**H bond donors**	0	**ACD/LogP**	2.99
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.16 g/cm^3
SMILES	Clc1cc(OC)cc(OC)c1				
STD InChIKey	WQHNWJBSROXROL-UHFFFAOYAD				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
34.00	Alfa Aesar
35.00	PHYSPROP

5-chloro-2-hydroxyaniline C6H6ClNO[2, 3, 64]

Compound Data



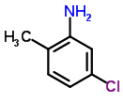
Melting point	**141.00 °C**	**414.15 K**			
CSID	6995	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	143.5709	**H bond donors**	3	**ACD/LogP**	1.67
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Clc1cc(N)c(O)cc1				
STD InChIKey	SWFNPENEBHAHEB-UHFFFAOYAR				

Melting Points

mp °C	source
143.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
140.00	Alfa Aesar
140.00	PHYSPROP

5-chloro-2-methylaniline C7H8ClN[3, 64]

Compound Data



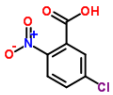
Melting point	**24.50 °C**	**297.65 K**			
CSID	6990	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	141.5981	**H bond donors**	2	**ACD/LogP**	2.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.18 g/cm^3
SMILES	Clc1cc(N)c(cc1)C				
STD InChIKey	WRZOMWDJOLIVQP-UHFFFAOYAU				

Melting Points

mp °C	source
23.00	Alfa Aesar
26.00	PHYSPROP

5-chloro-2-nitrobenzoic acid C7H4ClNO4[3, 64]

Compound Data



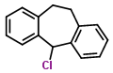
Melting point	**138.50 °C**	**411.65 K**			
CSID	16358	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.564	**H bond donors**	1	**ACD/LogP**	2.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	O=[N+]([O-])c1c(cc(Cl)cc1)C(=O)O				
STD InChIKey	ZKUYSJHXBFFGPU-UHFFFAOYAZ				

Melting Points

mp °C	source
138.00	Alfa Aesar
139.00	PHYSPROP

5-chlorodibenzosuberane C15H13Cl[3, 64]

Compound Data



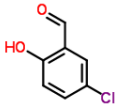
Melting point	**106.75 °C**	**379.90 K**			
CSID	13925	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	228.7167	**H bond donors**	0	**ACD/LogP**	3.62
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1ccc2c(c1)CCc3ccccc3C2Cl				
STD InChIKey	QPERNSDCEUTOTE-UHFFFAOYAZ				

Melting Points

mp °C	source
107.00	Alfa Aesar
106.50	PHYSPROP

5-chlorosalicylaldehyde C7H5ClO2[3, 64]

Compound Data



Melting point	**100.65 °C**	**373.80 K**			
CSID	11971	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.5664	**H bond donors**	1	**ACD/LogP**	2.57
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.40 g/cm^3
SMILES	Clc1cc(C=O)c(O)cc1				
STD InChIKey	FUGKCSRLAQKUHG-UHFFFAOYAF				

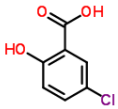
Melting Points

mp °C	source
101.00	Alfa Aesar
100.30	PHYSPROP

5-chlorosalicylic acid C7H5ClO3[2, 3, 64]

Compound Data

Melting point	**172.17 °C**	**445.32 K**			
CSID	9075	**H bond acceptors**	3	**Rule of 5 violations**	0



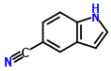
Molecular weight	172.5658	**H bond donors**	2	**ACD/LogP**	3.42
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.54 g/cm^3
SMILES	Clc1cc(C(=O)O)c(O)cc1				
STD InChIKey	NKBASRXWGAGQDP-UHFFFAOYAL				

Melting Points

mp °C	source
171.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
174.00	Alfa Aesar
171.50	PHYSPROP

5-cyanoindole C9H6N2[3, 64]

Compound Data



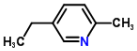
Melting point	**106.50 °C**	**379.65 K**			
CSID	25604	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	142.1573	**H bond donors**	1	**ACD/LogP**	2.36
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	N#Cc1cc2c(cc1)ncc2				
STD InChIKey	YHYLDEVWYOFIJK-UHFFFAOYAP				

Melting Points

mp °C	source
106.00	Alfa Aesar
107.00	PHYSPROP

5-ethyl-2-methylpyridine C8H11N[3, 61, 64]

Compound Data



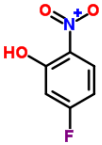
Melting point	**-70.97 °C**	**202.18 K**			
CSID	21105900	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.92 g/cm^3
SMILES	CCc1cnc(C)cc1				
STD InChIKey	NTSLROIKFLNUIJ-UHFFFAOYAH				

Melting Points

mp °C	source
-71.00	Alfa Aesar
-71.00	Oxford University MSDS
-70.90	PHYSPROP

5-fluoro-2-nitrophenol C6H4FNO3[3, 64]

Compound Data



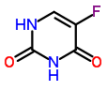
Melting point	**34.50 °C**	**307.65 K**			
CSID	9549	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	157.0993	**H bond donors**	1	**ACD/LogP**	1.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.51 g/cm^3
SMILES	O=[N+]([O-])c1ccc(F)cc1O				
STD InChIKey	QQURWFRNETXFTN-UHFFFAOYAE				

Melting Points

mp °C	source
33.00	Alfa Aesar
36.00	PHYSPROP

5-fluorouracil C4H3FN2O2[32, 44, 64]

Compound Data



Melting point	**282.00 °C**	**555.15 K**			
CSID	3268	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	130.0772	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.54 g/cm^3
SMILES	c1c(c(=O)[nH]c(=O)[nH]1)F				
STD InChIKey	GHASVSINZRGABV-UHFFFAOYAG				

Melting Points

mp °C	source
281.00	DrugBank
282.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
283.00	PHYSPROP

5-hydrofuran-2-one C4H4O2[3, 64]

Compound Data

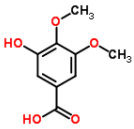
Melting point	**4.25 °C**	**277.40 K**			
CSID	9917	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	84.0734	**H bond donors**	0	**ACD/LogP**	-0.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.21 g/cm^3
SMILES	O=C\1OC/C=C/1				
STD InChIKey	VIHAEDVKXSOUAT-UHFFFAOYAD				

Melting Points

mp °C	source
4.00	Alfa Aesar
4.50	PHYSPROP

5-hydroxy-3,4-dimethoxybenzoic acid C9H10O5[3, 48]

Compound Data



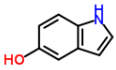
Melting point	**195.50 °C**	**468.65 K**			
CSID	67282	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	198.1727	**H bond donors**	2	**ACD/LogP**	1.50
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.33 g/cm^3
SMILES	O=C(O)c1cc(O)c(OC)c(OC)c1				
STD InChIKey	WFIBQVFJXGQICQ-UHFFFAOYAL				

Melting Points

mp °C	source
196.00	Alfa Aesar
195.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

5-hydroxyindole C8H7NO[3, 64]

Compound Data



Melting point	**108.25 °C**	**381.40 K**			
CSID	15244	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	133.1473	**H bond donors**	2	**ACD/LogP**	0.97
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	c1cc2c(cc[nH]2)cc1O				
STD InChIKey	LMIQERWZRIFWNZ-UHFFFAOYAS				

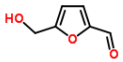
Melting Points

mp °C	source
109.00	Alfa Aesar
107.50	PHYSPROP

5-hydroxymethylfurfural C6H6O3[3, 64]

Compound Data

Melting point	**32.75 °C**	**305.90 K**	



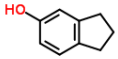
CSID	207215	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	126.11	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.29 g/cm^3
SMILES	c1cc(oc1CO)C=O				
STD InChIKey	NOEGNKMFWQHSLB-UHFFFAOYAB				

Melting Points

mp °C	source
34.00	Alfa Aesar
31.50	PHYSPROP

5-indanol C9H10O[3, 64]

Compound Data



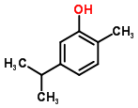
Melting point	**55.50 °C**	**328.65 K**			
CSID	14390	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	134.1751	**H bond donors**	1	**ACD/LogP**	2.60
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	Oc1ccc2c(c1)CCC2				
STD InChIKey	PEHSSTUGJUBZBI-UHFFFAOYAE				

Melting Points

mp °C	source
53.00	Alfa Aesar
58.00	PHYSPROP

5-isopropyl-2-methylphenol C10H14O[61, 64]

Compound Data



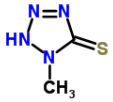
Melting point	**1.50 °C**	**274.65 K**			
CSID	21105867	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	1	**ACD/LogP**	3.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	Cc1ccc(cc1O)C(C)C				
STD InChIKey	RECUKUPTGUEGMW-UHFFFAOYAI				

Melting Points

mp °C	source
2.00	Oxford University MSDS
1.00	PHYSPROP

5-mercapto-1-methyltetrazole C2H4N4S[3, 48]

Compound Data



Melting point	**124.50 °C**	**397.65 K**			
CSID	2005963	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	116.145	**H bond donors**	1	**ACD/LogP**	-1.09
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.69 g/cm^3
SMILES	S=C1/N=N\NN1C				
STD InChIKey	XOHZHMUQBFJTNH-UHFFFAOYAZ				

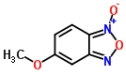
Melting Points

mp °C	source
127.00	Alfa Aesar
122.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

5-methoxybenzofuroxan C7H6N2O3[3, 48]

Compound Data

Melting point	**117.50 °C**	**390.65 K**			
CSID	284177	**H bond acceptors**	5	**Rule of 5 violations**	0



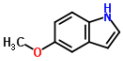
Molecular weight	166.1341	**H bond donors**	0	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	[O-][n+]1onc2cc(OC)ccc12				
STD InChIKey	ABSKHUSUHODMEL-UHFFFAOYAG				

Melting Points

mp °C	source
117.00	Alfa Aesar
118.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

5-methoxyindole C9H9NO[3, 64]

Compound Data



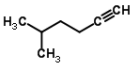
Melting point	**55.50 °C**	**328.65 K**			
CSID	13272	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	147.1739	**H bond donors**	1	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.17 g/cm^3
SMILES	COc1ccc2c(c1)cc[nH]2				
STD InChIKey	DWAQDRSOVMLGRQ-UHFFFAOYAJ				

Melting Points

mp °C	source
54.00	Alfa Aesar
57.00	PHYSPROP

5-methyl-1-hexyne C7H12[4, 64]

Compound Data



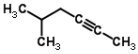
Melting point	**-124.50 °C**	**148.65 K**			
CSID	121154	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	2.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.75 g/cm^3
SMILES	C#CCCC(C)C				
STD InChIKey	HKNANEMUCJGPMS-UHFFFAOYAS				

Melting Points

mp °C	source
-124.00	American Petroleum Institute. Research Project 44; Selected ...
-125.00	PHYSPROP

5-methyl-2-hexyne C7H12[4, 64]

Compound Data



Melting point	**-92.95 °C**	**180.20 K**			
CSID	126201	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.75 g/cm^3
SMILES	C(#CCC(C)C)C				
STD InChIKey	SVGAHRUSRQTQES-UHFFFAOYAO				

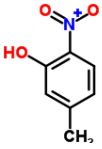
Melting Points

mp °C	source
-93.00	American Petroleum Institute. Research Project 44; Selected ...
-92.90	PHYSPROP

5-methyl-2-nitrophenol C7H7NO3[3, 64]

Compound Data

Melting point	**54.00 °C**	**327.15 K**			
CSID	12263	**H bond acceptors**	4	**Rule of 5 violations**	0

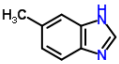


Molecular weight	153.1354	**H bond donors**	1	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	O=[N+]([O-])c1ccc(cc1O)C				
STD InChIKey	NQXUSSVLFOBRSE-UHFFFAOYAG				

Melting Points

mp °C	source
55.00	Alfa Aesar
53.00	PHYSPROP

5-methylbenzimidazole C8H8N2[3, 32, 64]



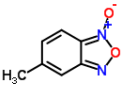
Compound Data

Melting point	**114.17 °C**	**387.32 K**			
CSID	11484	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	132.1625	**H bond donors**	1	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	n2c1ccc(cc1nc2)C				
STD InChIKey	RWXZXCZBMQPOBF-UHFFFAOYAW				

Melting Points

mp °C	source
115.00	Alfa Aesar
112.00	DrugBank
115.50	PHYSPROP

5-methylbenzofurazan N-oxide C7H6N2O2[3, 48]



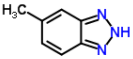
Compound Data

Melting point	**96.50 °C**	**369.65 K**			
CSID	123905	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	150.1347	**H bond donors**	0	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.40 g/cm^3
SMILES	[O-][n+]1onc2cc(ccc12)C				
STD InChIKey	HCWVKDOCXDWFEH-UHFFFAOYAO				

Melting Points

mp °C	source
97.00	Alfa Aesar
96.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

5-methylbenzotriazole C7H7N3[3, 61, 64]



Compound Data

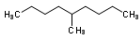
Melting point	**81.17 °C**	**354.32 K**			
CSID	8381	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	133.1506	**H bond donors**	1	**ACD/LogP**	1.60
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	n1c2ccc(cc2nn1)C				
STD InChIKey	LRUDIIUSNGCQKF-UHFFFAOYAO				

Melting Points

mp °C	source
81.00	Alfa Aesar
81.50	Oxford University MSDS
81.00	PHYSPROP

5-methylnonane C10H22[4, 64]

Compound Data



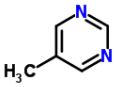
Melting point	**-87.85 °C**	**185.30 K**			
CSID	25609	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.73 g/cm^3
SMILES	CCCCC(CCCC)C				
STD InChIKey	TYSIILFJZXHVPU-UHFFFAOYAA				

Melting Points

mp °C	source
-88.00	American Petroleum Institute. Research Project 44; Selected ...
-87.70	PHYSPROP

5-methylpyrimidine C5H6N2[3, 64, 64]

Compound Data



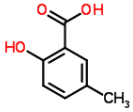
Melting point	**30.83 °C**	**303.98 K**			
CSID	67424	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.1145	**H bond donors**	0	**ACD/LogP**	0.01
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.02 g/cm^3
SMILES	Cc1cncnc1				
STD InChIKey	TWGNOYAGHYUFFR-UHFFFAOYAP				

Melting Points

mp °C	source
30.00	Alfa Aesar
32.00	PHYSPROP
30.50	PHYSPROP

5-methylsalicylic acid C8H8O3[3, 64]

Compound Data



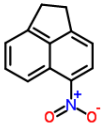
Melting point	**152.00 °C**	**425.15 K**			
CSID	6707	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	2	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.30 g/cm^3
SMILES	O=C(O)c1cc(ccc1O)C				
STD InChIKey	DLGBEGBHXSAQOC-UHFFFAOYAZ				

Melting Points

mp °C	source
153.00	Alfa Aesar
151.00	PHYSPROP

5-nitro-1,2-dihydroacenaphthylene C12H9NO2[61, 64]

Compound Data



Melting point	**103.25 °C**	**376.40 K**			
CSID	11276	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	199.2054	**H bond donors**	0	**ACD/LogP**	3.92
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	[O-][N+](=O)c1ccc3c2c1cccc2CC3				
STD InChIKey	CUARLQDWYSRQDF-UHFFFAOYAL				

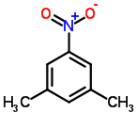
Melting Points

mp °C	source
103.50	Oxford University MSDS
103.00	PHYSPROP

5-nitro-1,3-dimethylbenzene C8H9NO2[2, 3, 64]

Compound Data

Melting point	**73.33 °C**	**346.48 K**	



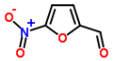
CSID	7148	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.13 g/cm^3
SMILES	[O-][N+](=O)c1cc(cc(c1)C)C				
STD InChIKey	BYFNZOKBMZKTSC-UHFFFAOYAW				

Melting Points

mp °C	source
74.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
71.00	Alfa Aesar
75.00	PHYSPROP

5-nitro-2-furaldehyde C5H3NO4[3, 64]

Compound Data



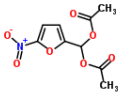
Melting point	**35.75 °C**	**308.90 K**			
CSID	12249	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	141.0816	**H bond donors**	0	**ACD/LogP**	0.51
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	O=Cc1oc([N+](=O)[O-])cc1				
STD InChIKey	SXINBFXPADXIEY-UHFFFAOYAX				

Melting Points

mp °C	source
36.00	Alfa Aesar
35.50	PHYSPROP

5-nitro-2-furaldehyde diacetate C9H9NO7[3, 64]

Compound Data



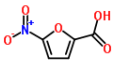
Melting point	**90.50 °C**	**363.65 K**			
CSID	6830	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	243.1703	**H bond donors**	0	**ACD/LogP**	0.18
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.40 g/cm^3
SMILES	O=[N+]([O-])c1oc(cc1)C(OC(=O)C)OC(=O)C				
STD InChIKey	HSXKWKJCZNRMJO-UHFFFAOYAS				

Melting Points

mp °C	source
90.00	Alfa Aesar
91.00	PHYSPROP

5-nitro-2-furoic acid C5H3NO5[3, 48, 64]

Compound Data



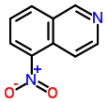
Melting point	**185.67 °C**	**458.82 K**			
CSID	12057	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	157.08	**H bond donors**	1	**ACD/LogP**	0.23
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.63 g/cm^3
SMILES	c1cc(oc1C(=O)O)[N+](=O)[O-]				
STD InChIKey	IODMEDPPCXSFLD-UHFFFAOYAZ				

Melting Points

mp °C	source
187.00	Alfa Aesar
184.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
186.00	PHYSPROP

5-nitroisoquinoline C9H6N2O2[3, 64]

Compound Data



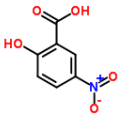
Melting point	**109.00 °C**	**382.15 K**			
CSID	62303	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1561	**H bond donors**	0	**ACD/LogP**	1.69
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	[O-][N+](=O)c1cccc2c1ccnc2				
STD InChIKey	PYGMPFQCCWBTJQ-UHFFFAOYAT				

Melting Points

mp °C	source
108.00	Alfa Aesar
110.00	PHYSPROP

5-nitrosalicylic acid C7H5NO5[3, 64]

Compound Data



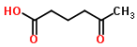
Melting point	**230.75 °C**	**503.90 K**			
CSID	7042	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	183.1183	**H bond donors**	2	**ACD/LogP**	2.35
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.63 g/cm^3
SMILES	O=C(O)c1cc(ccc1O)[N+]([O-])=O				
STD InChIKey	PPDRLQLKHRZIJC-UHFFFAOYAT				

Melting Points

mp °C	source
232.00	Alfa Aesar
229.50	PHYSPROP

5-oxohexanoic acid C6H10O3[3, 64]

Compound Data



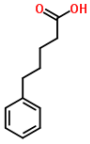
Melting point	**12.75 °C**	**285.90 K**			
CSID	17383	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	130.1418	**H bond donors**	1	**ACD/LogP**	-0.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	O=C(C)CCCC(=O)O				
STD InChIKey	MGTZCLMLSSAXLD-UHFFFAOYAE				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.50	PHYSPROP

5-phenylvaleric acid C11H14O2[3, 64]

Compound Data



Melting point	**58.25 °C**	**331.40 K**			
CSID	15886	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	178.2277	**H bond donors**	1	**ACD/LogP**	2.70
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.07 g/cm^3
SMILES	O=C(O)CCCCc1ccccc1				
STD InChIKey	BYHDDXPKOZIZRV-UHFFFAOYAD				

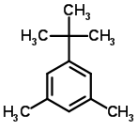
Melting Points

mp °C	source
59.00	Alfa Aesar
57.50	PHYSPROP

5-t-butyl-1,3-dimethylbenzene C12H18[3, 64]

Compound Data

Melting point	**-20.00 °C**	**253.15 K**			
CSID	7100	**H bond acceptors**	0	**Rule of 5 violations**	0



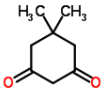
Molecular weight	162.2713	**H bond donors**	0	**ACD/LogP**	4.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.86 g/cm^3
SMILES	c1c(cc(cc1C(C)(C)C)C)C				
STD InChIKey	FZSPYHREEHYLCB-UHFFFAOYAL				

Melting Points

mp °C	source
-22.00	Alfa Aesar
-18.00	PHYSPROP

5,5-dimethylcyclohexane-1,3-dione C8H12O2[3, 61]

Compound Data



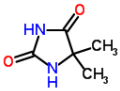
Melting point	**148.25 °C**	**421.40 K**			
CSID	29091	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	140.1797	**H bond donors**	0	**ACD/LogP**	0.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.02 g/cm^3
SMILES	O=C1CC(=O)CC(C)(C)C1				
STD InChIKey	BADXJIPKFRBFOT-UHFFFAOYAX				

Melting Points

mp °C	source
148.00	Alfa Aesar
148.50	Oxford University MSDS

5,5-dimethylhydantoin C5H8N2O2[3, 64]

Compound Data



Melting point	**177.00 °C**	**450.15 K**			
CSID	6246	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	128.1292	**H bond donors**	2	**ACD/LogP**	-0.66
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	O=C1NC(=O)NC1(C)C				
STD InChIKey	YIROYDNZEPTFOL-UHFFFAOYAJ				

Melting Points

mp °C	source
176.00	Alfa Aesar
178.00	PHYSPROP

5,5-dimethyloxazolidine-2,4-dione C5H7NO3[3, 64]

Compound Data

Melting point	**77.75 °C**	**350.90 K**			
CSID	2972	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	129.114	**H bond donors**	1	**ACD/LogP**	0.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	O=C1NC(=O)OC1(C)C				
STD InChIKey	JYJFNDQBESEHJQ-UHFFFAOYAJ				

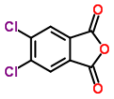
Melting Points

mp °C	source
79.00	Alfa Aesar
76.50	PHYSPROP

5,6-dichloro-2-benzofuran-1,3-dione C8H2Cl2O3[48, 64]

Compound Data

Melting point	**187.00 °C**	**460.15 K**			
CSID	63515	**H bond acceptors**	3	**Rule of 5 violations**	0



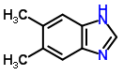
Molecular weight	217.0057	**H bond donors**	0	**ACD/LogP**	2.67
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.72 g/cm^3
SMILES	Clc1cc2C(=O)OC(=O)c2cc1Cl				
STD InChIKey	ULSOWUBMELTORB-UHFFFAOYAF				

Melting Points

mp °C	source
186.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
188.00	PHYSPROP

5,6-dimethylbenzimidazole C9H10N2[3, 32, 64]

Compound Data



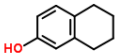
Melting point	**205.00 °C**	**478.15 K**			
CSID	655	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	146.1891	**H bond donors**	1	**ACD/LogP**	2.31
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.15 g/cm^3
SMILES	n2c1cc(c(cc1nc2)C)C				
STD InChIKey	LJUQGASMPRMWIW-UHFFFAOYAV				

Melting Points

mp °C	source
204.00	Alfa Aesar
205.50	DrugBank
205.50	PHYSPROP

5,6,7,8-tetrahydro-2-naphthol C10H12O[3, 64]

Compound Data



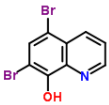
Melting point	**59.50 °C**	**332.65 K**			
CSID	13667	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	148.2017	**H bond donors**	1	**ACD/LogP**	3.17
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.10 g/cm^3
SMILES	Oc1ccc2c(c1)CCCC2				
STD InChIKey	UMKXSOXZAXIOPJ-UHFFFAOYAJ				

Melting Points

mp °C	source
62.00	Alfa Aesar
57.00	PHYSPROP

5,7-dibromo-8-hydroxyquinoline C9H5Br2NO[3, 64]

Compound Data



Melting point	**198.50 °C**	**471.65 K**			
CSID	2359	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	302.9501	**H bond donors**	1	**ACD/LogP**	3.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.05 g/cm^3
SMILES	Brc1c(O)c2ncccc2c(Br)c1				
STD InChIKey	ZDASUJMDVPTNTF-UHFFFAOYAL				

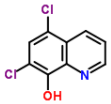
Melting Points

mp °C	source
201.00	Alfa Aesar
196.00	PHYSPROP

5,7-dichloro-8-hydroxyquinoline C9H5Cl2NO[3, 32, 64]

Compound Data

Melting point	**180.00 °C**	**453.15 K**



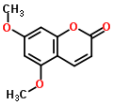
CSID	2621	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	214.0481	**H bond donors**	1	**ACD/LogP**	3.75
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	Clc1c(O)c2ncccc2c(Cl)c1				
STD InChIKey	WDFKMLRRRCGAKS-UHFFFAOYAZ				

Melting Points

mp °C	source
181.00	Alfa Aesar
179.50	DrugBank
179.50	PHYSPROP

5,7-dimethoxycoumarin C11H10O4[3, 64]

Compound Data



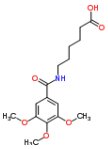
Melting point	**148.50 °C**	**421.65 K**			
CSID	2673	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	206.1947	**H bond donors**	0	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	O=C/2Oc1cc(OC)cc(OC)c1\C=C\2				
STD InChIKey	NXJCRELRQHZBQA-UHFFFAOYAC				

Melting Points

mp °C	source
148.00	Alfa Aesar
149.00	PHYSPROP

6-(3,4,5-trimethoxybenzamido)hexanoic acid C16H23NO6[9, 48, 64]

Compound Data



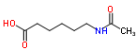
Melting point	**121.33 °C**	**394.48 K**			
CSID	28425	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	325.3569	**H bond donors**	2	**ACD/LogP**	0.54
Phase 25 °C	solid	**Rotatable bonds**	10	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)CCCCCNC(=O)c1cc(OC)c(OC)c(OC)c1				
STD InChIKey	MPTXLVRHYGBOQY-UHFFFAOYAV				

Melting Points

mp °C	source
121.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
121.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
122.00	PHYSPROP

6-acetamidohexanoic acid C8H15NO3[3, 64]

Compound Data



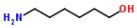
Melting point	**104.25 °C**	**377.40 K**			
CSID	1928	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	173.2096	**H bond donors**	2	**ACD/LogP**	-0.50
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.07 g/cm^3
SMILES	O=C(NCCCCCC(=O)O)C				
STD InChIKey	WDSCBUNMANHPFH-UHFFFAOYAB				

Melting Points

mp °C	source
104.00	Alfa Aesar
104.50	PHYSPROP

6-amino-1-hexanol C6H15NO[2, 3, 61, 64]

Compound Data



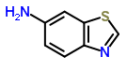
Melting point	**56.50 °C**	**329.65 K**			
CSID	18801	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	117.1894	**H bond donors**	3	**ACD/LogP**	-0.01
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	0.91 g/cm^3
SMILES	OCCCCCCN				
STD InChIKey	SUTWPJHCRAITLU-UHFFFAOYAA				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
57.00	Alfa Aesar
56.00	Oxford University MSDS
57.00	PHYSPROP

6-aminobenzothiazole C7H6N2S[3, 64]

Compound Data



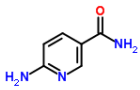
Melting point	**87.50 °C**	**360.65 K**			
CSID	61585	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.2009	**H bond donors**	2	**ACD/LogP**	0.73
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.38 g/cm^3
SMILES	n1c2ccc(cc2sc1)N				
STD InChIKey	FAYAYUOZWYJNBD-UHFFFAOYAX				

Melting Points

mp °C	source
88.00	Alfa Aesar
87.00	PHYSPROP

6-aminonicotinamide C6H7N3O[3, 64]

Compound Data



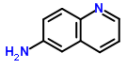
Melting point	**246.75 °C**	**519.90 K**			
CSID	9128	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	137.1393	**H bond donors**	4	**ACD/LogP**	0.41
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	O=C(c1cnc(N)cc1)N				
STD InChIKey	ZLWYEPMDOUQDBW-UHFFFAOYAD				

Melting Points

mp °C	source
247.00	Alfa Aesar
246.50	PHYSPROP

6-aminoquinoline C9H8N2[3, 64]

Compound Data



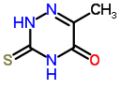
Melting point	**115.50 °C**	**388.65 K**			
CSID	10895	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.1732	**H bond donors**	2	**ACD/LogP**	1.26
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	n1cccc2cc(ccc12)N				
STD InChIKey	RJSRSRITMWVIQT-UHFFFAOYAK				

Melting Points

mp °C	source
117.00	Alfa Aesar
114.00	PHYSPROP

6-aza-2-thiothymine C4H5N3OS[3, 64]

Compound Data



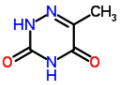
Melting point	**219.25 °C**	**492.40 K**			
CSID	1061203	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	143.167	**H bond donors**	2	**ACD/LogP**	-1.46
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.63 g/cm^3
SMILES	O=C1\C(=N/NC(=S)N1)C				
STD InChIKey	NKOPQOSBROLOFP-UHFFFAOYAI				

Melting Points

mp °C	source
220.00	Alfa Aesar
218.50	PHYSPROP

6-azathymine C4H5N3O2[3, 64]

Compound Data



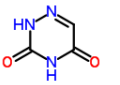
Melting point	**212.00 °C**	**485.15 K**			
CSID	63453	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	127.1014	**H bond donors**	2	**ACD/LogP**	-0.31
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.67 g/cm^3
SMILES	O=C1\C(=N/NC(=O)N1)C				
STD InChIKey	XZWMZFQOHTWGQE-UHFFFAOYAT				

Melting Points

mp °C	source
213.00	Alfa Aesar
211.00	PHYSPROP

6-azauracil C3H3N3O2[3, 64]

Compound Data



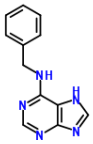
Melting point	**275.25 °C**	**548.40 K**			
CSID	61352	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	113.0748	**H bond donors**	2	**ACD/LogP**	-0.59
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.86 g/cm^3
SMILES	O=C1\C=N/NC(=O)N1				
STD InChIKey	SSPYSWLZOPCOLO-UHFFFAOYAO				

Melting Points

mp °C	source
276.00	Alfa Aesar
274.50	PHYSPROP

6-benzylaminopurine C12H11N5[3, 61, 64]

Compound Data



Melting point	**232.17 °C**	**505.32 K**			
CSID	56177	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	225.2492	**H bond donors**	2	**ACD/LogP**	0.54
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	n1c(c2c(nc1)ncn2)NCc3ccccc3				
STD InChIKey	NWBJYWHLCVSVIJ-UHFFFAOYAZ				

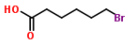
Melting Points

mp °C	source
231.00	Alfa Aesar
231.00	Oxford University MSDS
234.50	PHYSPROP

6-bromohexanoic acid C6H11BrO2[3, 64]

Compound Data

Melting point	**34.50 °C**	**307.65 K**



CSID	19037	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	195.0543	**H bond donors**	1	**ACD/LogP**	1.70
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.44 g/cm^3
SMILES	BrCCCCCC(=O)O				
STD InChIKey	NVRVNSHHLPQGCU-UHFFFAOYAQ				

Melting Points

mp °C	source
34.00	Alfa Aesar
35.00	PHYSPROP

6-chloro-2,4-dinitroaniline C6H4ClN3O4[2, 3]

Compound Data

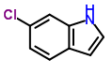
Melting point	**155.50 °C**	**428.65 K**			
CSID	17987	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	217.5667	**H bond donors**	2	**ACD/LogP**	3.38
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.71 g/cm^3
SMILES	Clc1cc(cc([N+]([O-])=O)c1N)[N+]([O-])=O				
STD InChIKey	LHRIICYSGQGXSX-UHFFFAOYAO				

Melting Points

mp °C	source
157.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
154.00	Alfa Aesar

6-chloroindole C8H6ClN[3, 64]

Compound Data



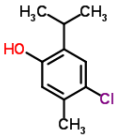
Melting point	**89.50 °C**	**362.65 K**			
CSID	78578	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	151.5929	**H bond donors**	1	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.33 g/cm^3
SMILES	Clc1ccc2c(c1)ncc2				
STD InChIKey	YTYIMDRWPTUAHP-UHFFFAOYAC				

Melting Points

mp °C	source
89.00	Alfa Aesar
90.00	PHYSPROP

6-chorothymol C10H13ClO[3, 61, 64]

Compound Data



Melting point	**60.67 °C**	**333.82 K**			
CSID	6716	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.6626	**H bond donors**	1	**ACD/LogP**	4.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	Clc1cc(c(O)cc1C)C(C)C				
STD InChIKey	KFZXVMNBUMVKLN-UHFFFAOYAM				

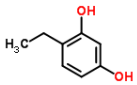
Melting Points

mp °C	source
60.00	Alfa Aesar
59.00	Oxford University MSDS
63.00	PHYSPROP

6-ethylresorcinol C8H10O2[3, 64]

Compound Data

Melting point	**97.75 °C**	**370.90 K**

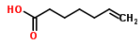


CSID	16931	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	2	**ACD/LogP**	1.75
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	Oc1cc(O)ccc1CC				
STD InChIKey	VGMJYYDKPUPTID-UHFFFAOYAW				

Melting Points

mp °C	source
97.00	Alfa Aesar
98.50	PHYSPROP

6-heptenoic acid C7H12O2[3, 64]



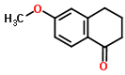
Compound Data

Melting point	**-6.25 °C**	**266.90 K**			
CSID	63871	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.169	**H bond donors**	1	**ACD/LogP**	1.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.96 g/cm^3
SMILES	O=C(O)CCCC\C=C				
STD InChIKey	RWNJOXUVHRXHSD-UHFFFAOYAN				

Melting Points

mp °C	source
-6.00	Alfa Aesar
-6.50	PHYSPROP

6-methoxy-1-tetralone C11H12O2[3, 64]



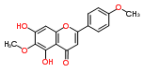
Compound Data

Melting point	**78.50 °C**	**351.65 K**			
CSID	13490	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	176.2118	**H bond donors**	0	**ACD/LogP**	2.69
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	O=C2c1c(cc(OC)cc1)CCC2				
STD InChIKey	MNALUTYMBUBKNX-UHFFFAOYAS				

Melting Points

mp °C	source
79.00	Alfa Aesar
78.00	PHYSPROP

6-methoxyacacetin C17H14O6[47, 64]



Compound Data

Melting point	**223.00 °C**	**496.15 K**			
CSID	4478521	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	314.2895	**H bond donors**	2	**ACD/LogP**	2.64
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.40 g/cm^3
SMILES	O=C\1c3c(O)c(OC)c(O)cc3O/C(=C/1)c2ccc(OC)cc2				
STD InChIKey	GPQLHGCIAUEJQK-UHFFFAOYAB				

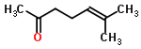
Melting Points

mp °C	source
225.00	IUCr
221.00	PHYSPROP

6-methyl-5-hepten-2-one C8H14O[3, 64]

Compound Data

Melting point	**-67.05 °C**	**206.10 K**			
CSID	9478	**H bond acceptors**	1	**Rule of 5 violations**	0



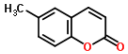
Molecular weight	126.1962	**H bond donors**	0	**ACD/LogP**	2.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.83 g/cm^3
SMILES	O=C(C)CC\C=C(/C)C				
STD InChIKey	UHEPJGULSIKKTP-UHFFFAOYAX				

Melting Points

mp °C	source
-67.00	Alfa Aesar
-67.10	PHYSPROP

6-methylcoumarin C10H8O2[3, 64]

Compound Data



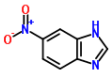
Melting point	**76.25 °C**	**349.40 K**			
CSID	6825	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.1693	**H bond donors**	0	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	O=C/2Oc1ccc(cc1\C=C\2)C				
STD InChIKey	FXFYOPQLGGEACP-UHFFFAOYAB				

Melting Points

mp °C	source
76.00	Alfa Aesar
76.50	PHYSPROP

6-nitrobenzimidazole C7H5N3O2[3, 61, 64]

Compound Data



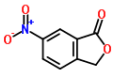
Melting point	**208.33 °C**	**481.48 K**			
CSID	6927	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	163.1335	**H bond donors**	1	**ACD/LogP**	1.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	[O-][N+](=O)c1ccc2ncnc2c1				
STD InChIKey	XPAZGLFMMUODDK-UHFFFAOYAW				

Melting Points

mp °C	source
209.00	Alfa Aesar
208.00	Oxford University MSDS
208.00	PHYSPROP

6-nitrophthalide C8H5NO4[3, 64]

Compound Data



Melting point	**144.00 °C**	**417.15 K**			
CSID	194210	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	179.1296	**H bond donors**	0	**ACD/LogP**	0.61
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.52 g/cm^3
SMILES	[O-][N+](=O)c1cc2C(=O)OCc2cc1				
STD InChIKey	RNWGZXAHUPFXLL-UHFFFAOYAN				

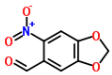
Melting Points

mp °C	source
143.00	Alfa Aesar
145.00	PHYSPROP

6-nitropiperonal C8H5NO5[3, 64]

Compound Data

Melting point	**94.25 °C**	**367.40 K**	



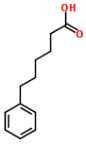
CSID	12310	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	195.129	**H bond donors**	0	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.57 g/cm^3
SMILES	[O-][N+](=O)c1c(cc2OCOc2c1)C=O				
STD InChIKey	NRZWECORTTWSEF-UHFFFAOYAY				

Melting Points

mp °C	source
95.00	Alfa Aesar
93.50	PHYSPROP

6-phenylhexanoic acid C12H16O2[3, 64]

Compound Data



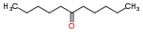
Melting point	**20.50 °C**	**293.65 K**			
CSID	71995	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	192.2542	**H bond donors**	1	**ACD/LogP**	3.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	1.05 g/cm^3
SMILES	O=C(O)CCCCCc1ccccc1				
STD InChIKey	JTXZPQIXIXYMDY-UHFFFAOYAZ				

Melting Points

mp °C	source
18.00	Alfa Aesar
23.00	PHYSPROP

6-undecanone C11H22O[2, 64]

Compound Data



Melting point	**14.75 °C**	**287.90 K**			
CSID	12972	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2918	**H bond donors**	0	**ACD/LogP**	4.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.82 g/cm^3
SMILES	O=C(CCCCC)CCCCC				
STD InChIKey	ZPQAKYPOZRXKFA-UHFFFAOYAY				

Melting Points

mp °C	source
15.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
14.50	PHYSPROP

7-azaindole C7H6N2[3, 64]

Compound Data

Melting point	**105.50 °C**	**378.65 K**			
CSID	8867	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1359	**H bond donors**	1	**ACD/LogP**	1.82
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	c1cc2cc[nH]c2nc1				
STD InChIKey	MVXVYAKCVDQRLW-UHFFFAOYAE				

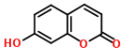
Melting Points

mp °C	source
105.00	Alfa Aesar
106.00	PHYSPROP

7-hydroxycoumarin C9H6O3[3, 64]

Compound Data

Melting point	**230.25 °C**	**503.40 K**			
CSID	4444774	**H bond acceptors**	3	**Rule of 5 violations**	0



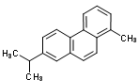
Molecular weight	162.1421	**H bond donors**	1	**ACD/LogP**	1.58
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	c1cc(cc2c1ccc(=O)o2)O				
STD InChIKey	ORHBXUUXSCNDEV-UHFFFAOYAL				

Melting Points

mp °C	source
230.00	Alfa Aesar
230.50	PHYSPROP

7-isopropyl-1-methylphenanthrene C18H18[61, 64]

Compound Data



Melting point	**100.00 °C**	**373.15 K**			
CSID	9805	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	234.3355	**H bond donors**	0	**ACD/LogP**	6.49
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	Cc1cccc2c1ccc3c2ccc(c3)C(C)C				
STD InChIKey	NXLOLUFNDSBYTP-UHFFFAOYAL				

Melting Points

mp °C	source
99.00	Oxford University MSDS
101.00	PHYSPROP

7-methylindole C9H8N[3, 64]

Compound Data

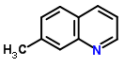
Melting point	**84.50 °C**	**357.65 K**			
CSID	63459	**H bond acceptors**	NA	**Rule of 5 violations**	NA
Molecular weight	130.1665	**H bond donors**	NA	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	NA	**Predicted density**	0.00 g/cm^3
SMILES	Cc1cccc2c1[nH]cc2				
STD InChIKey	KGWPHCDTOLQQEP-UHFFFAOYAX				

Melting Points

mp °C	source
84.00	Alfa Aesar
85.00	PHYSPROP

7-methylquinoline C10H9N[61, 64]

Compound Data



Melting point	**37.75 °C**	**310.90 K**			
CSID	11433	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	n1cccc2ccc(cc12)C				
STD InChIKey	KDYVCOSVYOSHOL-UHFFFAOYAQ				

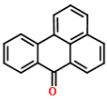
Melting Points

mp °C	source
36.50	Oxford University MSDS
39.00	PHYSPROP

7-oxobenz[de]anthracene C17H10O[3, 61, 64]

Compound Data

Melting point	**171.00 °C**	**444.15 K**			
CSID	6442	**H bond acceptors**	1	**Rule of 5 violations**	0



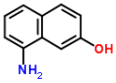
Molecular weight	230.2607	**H bond donors**	0	**ACD/LogP**	4.81
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	O=C3c4c(c2cccc1cccc3c12)cccc4				
STD InChIKey	HUKPVYBUJRAUAG-UHFFFAOYAL				

Melting Points

mp °C	source
173.00	Alfa Aesar
170.00	Oxford University MSDS
170.00	PHYSPROP

8-amino-2-naphthol C10H9NO[3, 64]

Compound Data



Melting point	**207.00 °C**	**480.15 K**			
CSID	8055	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	159.1846	**H bond donors**	3	**ACD/LogP**	1.43
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	Oc2ccc1c(c(ccc1)N)c2				
STD InChIKey	KVHHMYZBFBSVDI-UHFFFAOYAQ				

Melting Points

mp °C	source
208.00	Alfa Aesar
206.00	PHYSPROP

8-aminoquinoline C9H8N2[3, 64]

Compound Data

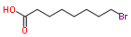
Melting point	**67.50 °C**	**340.65 K**			
CSID	10881	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.1732	**H bond donors**	2	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	n1cccc2cccc(N)c12				
STD InChIKey	WREVVZMUNPAPOV-UHFFFAOYAR				

Melting Points

mp °C	source
65.00	Alfa Aesar
70.00	PHYSPROP

8-bromooctanoic acid C8H15BrO2[3, 35, 64]

Compound Data



Melting point	**38.67 °C**	**311.82 K**			
CSID	477171	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	223.1075	**H bond donors**	1	**ACD/LogP**	2.76
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.32 g/cm^3
SMILES	BrCCCCCCCC(=O)O				
STD InChIKey	BKJFDZSBZWHRNH-UHFFFAOYAK				

Melting Points

mp °C	source
39.00	Alfa Aesar
38.50	EPISuite-ChemSpider
38.50	PHYSPROP

8-hydroxy-2-methylquinoline C10H9NO[3, 64]

Compound Data

Melting point	**72.90 °C**	**346.05 K**			
CSID	12669	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	159.1846	**H bond donors**	1	**ACD/LogP**	2.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	Oc1cccc2ccc(nc12)C				
STD InChIKey	NBYLBWHHTUWMER-UHFFFAOYAF				

Melting Points

mp °C	source
72.00	Alfa Aesar
73.80	PHYSPROP

8-hydroxyquinoline C9H7NO[3, 61, 64]

Compound Data

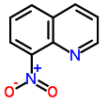
Melting point	**75.17 °C**	**348.32 K**			
CSID	1847	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	145.158	**H bond donors**	1	**ACD/LogP**	1.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	c1cc2cccnc2c(c1)O				
STD InChIKey	MCJGNVYPOGVAJF-UHFFFAOYAG				

Melting Points

mp °C	source
74.00	Alfa Aesar
76.00	Oxford University MSDS
75.50	PHYSPROP

8-nitroquinoline C9H6N2O2[3, 64]

Compound Data



Melting point	**89.00 °C**	**362.15 K**			
CSID	11337	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1561	**H bond donors**	0	**ACD/LogP**	1.47
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	[O-][N+](=O)c1cccc2cccnc12				
STD InChIKey	OQHHSGRZCKGLCY-UHFFFAOYAK				

Melting Points

mp °C	source
88.00	Alfa Aesar
90.00	PHYSPROP

9-bromofluorene C13H9Br[3, 64]

Compound Data

Melting point	**103.25 °C**	**376.40 K**			
CSID	15216	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	245.1146	**H bond donors**	0	**ACD/LogP**	4.28
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.51 g/cm^3
SMILES	BrC3c1ccccc1c2c3cccc2				
STD InChIKey	AHCDKANCCBEQJJ-UHFFFAOYAL				

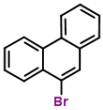
Melting Points

mp °C	source
103.00	Alfa Aesar
103.50	PHYSPROP

9-bromophenanthrene C14H9Br[3, 64]

Compound Data

Melting point	**64.25 °C**	**337.40 K**			



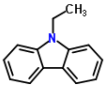
CSID	10834	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	257.1253	**H bond donors**	0	**ACD/LogP**	5.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.48 g/cm^3
SMILES	Brc2cc3c(c1c2cccc1)cccc3				
STD InChIKey	RSQXKVWKJVUZDG-UHFFFAOYAG				

Melting Points

mp °C	source
64.00	Alfa Aesar
64.50	PHYSPROP

9-ethylcarbazole C14H13N[3, 61, 64]

Compound Data



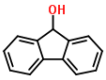
Melting point	**68.67 °C**	**341.82 K**			
CSID	6575	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	195.2597	**H bond donors**	0	**ACD/LogP**	4.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	c1cccc3c1c2c(cccc2)n3CC				
STD InChIKey	PLAZXGNBGZYJSA-UHFFFAOYAZ				

Melting Points

mp °C	source
69.00	Alfa Aesar
69.00	Oxford University MSDS
68.00	PHYSPROP

9-fluorenol C13H10O[3, 61, 64]

Compound Data



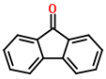
Melting point	**154.33 °C**	**427.48 K**			
CSID	66916	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.2179	**H bond donors**	1	**ACD/LogP**	2.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	OC3c1ccccc1c2c3cccc2				
STD InChIKey	AFMVESZOYKHDBJ-UHFFFAOYAM				

Melting Points

mp °C	source
156.00	Alfa Aesar
153.50	Oxford University MSDS
153.50	PHYSPROP

9-fluorenone C13H8O[3, 35, 61, 64]

Compound Data

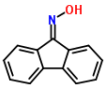


Melting point	**83.75 °C**	**356.90 K**			
CSID	9824	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	180.202	**H bond donors**	0	**ACD/LogP**	3.49
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	c1ccc2c(c1)-c3ccccc3C2=O				
STD InChIKey	YLQWCDOCJODRMT-UHFFFAOYAR				

Melting Points

mp °C	source
84.00	Alfa Aesar
84.00	EPISuite-ChemSpider
83.00	Oxford University MSDS
84.00	PHYSPROP

9-fluorenone oxime C13H9NO[3, 64]



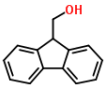
Compound Data

Melting point	**194.75 °C**	**467.90 K**			
CSID	15683	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	195.2167	**H bond donors**	1	**ACD/LogP**	3.39
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	O\N=C3/c1ccccc1c2c3cccc2				
STD InChIKey	CRNNFEKVPRFZKJ-UHFFFAOYAD				

Melting Points

mp °C	source
194.00	Alfa Aesar
195.50	PHYSPROP

9-fluorenylmethanol C14H12O[3, 64]



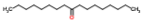
Compound Data

Melting point	**105.00 °C**	**378.15 K**			
CSID	81679	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.2445	**H bond donors**	1	**ACD/LogP**	3.33
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	OCC3c1ccccc1c2c3cccc2				
STD InChIKey	XXSCONYSQQLHTH-UHFFFAOYAS				

Melting Points

mp °C	source
104.00	Alfa Aesar
106.00	PHYSPROP

9-heptadecanone C17H34O[3, 64]



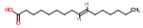
Compound Data

Melting point	**52.50 °C**	**325.65 K**			
CSID	10425	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	254.4513	**H bond donors**	0	**ACD/LogP**	7.28
Phase 25 °C	solid	**Rotatable bonds**	14	**Predicted density**	0.83 g/cm^3
SMILES	O=C(CCCCCCCC)CCCCCCCC				
STD InChIKey	WTJKUFMLQFLJOT-UHFFFAOYAB				

Melting Points

mp °C	source
52.00	Alfa Aesar
53.00	PHYSPROP

9-hexadecenoic acid C16H30O2[64, 64]



Compound Data

Melting point	**0.20 °C**	**273.35 K**			
CSID	4445872	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	254.4082	**H bond donors**	1	**ACD/LogP**	6.63
Phase 25 °C	liquid/gas	**Rotatable bonds**	13	**Predicted density**	0.91 g/cm^3
SMILES	O=C(O)CCCCCCC/C=C/CCCCCC				
STD InChIKey	SECPZKHBENQXJG-BQYQJAHWBY				

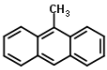
Melting Points

mp °C	source
0.50	PHYSPROP
-0.10	PHYSPROP

9-methylanthracene C15H12[3, 61, 64]

Compound Data

Melting point	**79.83 °C**	**352.98 K**



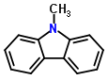
CSID	12524	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	192.2558	**H bond donors**	0	**ACD/LogP**	5.09
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.10 g/cm^3
SMILES	Cc1c2ccccc2cc3c1cccc3				
STD InChIKey	CPGPAVAKSZHMBP-UHFFFAOYAW				

Melting Points

mp °C	source
80.00	Alfa Aesar
78.00	Oxford University MSDS
81.50	PHYSPROP

9-methylcarbazole C13H11N[61, 64]

Compound Data



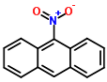
Melting point	**90.17 °C**	**363.32 K**			
CSID	14413	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	181.2331	**H bond donors**	0	**ACD/LogP**	3.99
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.09 g/cm^3
SMILES	c1cccc3c1c2c(cccc2)n3C				
STD InChIKey	SDFLTYHTFPTIGX-UHFFFAOYAX				

Melting Points

mp °C	source
91.00	Oxford University MSDS
89.34	PHYSPROP

9-nitroanthracene C14H9NO2[3, 64]

Compound Data



Melting point	**143.50 °C**	**416.65 K**			
CSID	11274	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	223.2268	**H bond donors**	0	**ACD/LogP**	4.41
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	[O-][N+](=O)c2c3c(cc1c2cccc1)cccc3				
STD InChIKey	LSIKFJXEYJIZNB-UHFFFAOYAH				

Melting Points

mp °C	source
141.00	Alfa Aesar
146.00	PHYSPROP

9-octadecynoic acid C18H32O2[3, 64]

Compound Data

Melting point	**46.50 °C**	**319.65 K**			
CSID	61475	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	280.4455	**H bond donors**	1	**ACD/LogP**	6.79
Phase 25 °C	solid	**Rotatable bonds**	14	**Predicted density**	0.92 g/cm^3
SMILES	O=C(O)CCCCCCCC#CCCCCCCCC				
STD InChIKey	RGTIBVZDHOMOKC-UHFFFAOYAM				

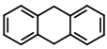
Melting Points

mp °C	source
45.00	Alfa Aesar
48.00	PHYSPROP

9,10-dihydroanthracene C14H12[48, 61, 64]

Compound Data

Melting point	**109.33 °C**	**382.48 K**



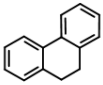
CSID	11446	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	180.2451	**H bond donors**	0	**ACD/LogP**	4.16
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	c1ccc3c(c1)Cc2c(cccc2)C3				
STD InChIKey	WPDAVTSOEQEGMS-UHFFFAOYAH				

Melting Points

mp °C	source
108.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
109.00	Oxford University MSDS
111.00	PHYSPROP

9,10-dihydrophenanthrene C14H12[48, 64]

Compound Data



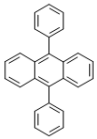
Melting point	**34.25 °C**	**307.40 K**			
CSID	12515	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	180.2451	**H bond donors**	0	**ACD/LogP**	5.04
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	c3ccc2c(c1c(cccc1)CC2)c3				
STD InChIKey	XXPBFNVKTVJZKF-UHFFFAOYAZ				

Melting Points

mp °C	source
34.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
34.50	PHYSPROP

9,10-diphenylanthracene C26H18[3, 61, 64]

Compound Data



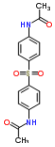
Melting point	**248.67 °C**	**521.82 K**			
CSID	14430	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	330.4211	**H bond donors**	0	**ACD/LogP**	8.46
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	c1ccc(cc1)c2c3ccccc3c(c4c2cccc4)c5ccccc5				
STD InChIKey	FCNCGHJSNVOIKE-UHFFFAOYAL				

Melting Points

mp °C	source
251.00	Alfa Aesar
249.00	Oxford University MSDS
246.00	PHYSPROP

acedapsone C16H16N2O4S[9, 64]

Compound Data



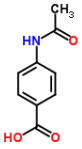
Melting point	**289.50 °C**	**562.65 K**			
CSID	6232	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	332.3742	**H bond donors**	2	**ACD/LogP**	1.53
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.36 g/cm^3
SMILES	O=S(=O)(c1ccc(NC(=O)C)cc1)c2ccc(NC(=O)C)cc2				
STD InChIKey	AMTPYFGPPVFBBI-UHFFFAOYAQ				

Melting Points

mp °C	source
289.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
290.00	PHYSPROP

acedoben C9H9NO3[2, 32, 35, 61]

Compound Data



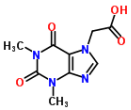
Melting point	**258.75 °C**	**531.90 K**			
CSID	18177	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	179.1727	**H bond donors**	2	**ACD/LogP**	1.31
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=C(Nc1ccc(cc1)C(=O)O)C				
STD InChIKey	QCXJEYYXVJIFCE-UHFFFAOYAT				

Melting Points

mp °C	source
259.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
260.00	DrugBank
260.00	EPISuite-ChemSpider
256.00	Oxford University MSDS

acefylline C9H10N4O4[3, 9, 48]

Compound Data



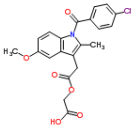
Melting point	**270.67 °C**	**543.82 K**			
CSID	62754	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	238.2001	**H bond donors**	1	**ACD/LogP**	-0.49
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.64 g/cm^3
SMILES	O=C2N(c1ncn(c1C(=O)N2C)CC(=O)O)C				
STD InChIKey	HCYFGRCYSCXKNQ-UHFFFAOYAG				

Melting Points

mp °C	source
270.00	Alfa Aesar
271.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
271.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

acemetacin C21H18ClNO6[9, 48, 64]

Compound Data



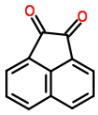
Melting point	**150.50 °C**	**423.65 K**			
CSID	1904	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	415.8237	**H bond donors**	1	**ACD/LogP**	3.20
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.36 g/cm^3
SMILES	Clc1ccc(cc1)C(=O)n3c2ccc(OC)cc2c(c3C)CC(=O)OCC(=O)O				
STD InChIKey	FSQKKOOTNAMONP-UHFFFAOYAI				

Melting Points

mp °C	source
150.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
150.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
151.50	PHYSPROP

acenaphthenequinone C12H6O2[3, 64]

Compound Data



Melting point	**259.50 °C**	**532.65 K**			
CSID	6468	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	182.1748	**H bond donors**	0	**ACD/LogP**	2.28
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	O=C3c2cccc1cccc(c12)C3=O				
STD InChIKey	AFPRJLBZLPBTPZ-UHFFFAOYAC				

Melting Points

mp °C	source
258.00	Alfa Aesar
261.00	PHYSPROP

acenaphthylene C12H8[61, 64]

Compound Data

Melting point	**91.75 °C**	**364.90 K**			
CSID	8807	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	152.1919	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1cc2cccc3c2c(c1)C=C3				
STD InChIKey	HXGDTGSAIMULJN-UHFFFAOYAQ				

Melting Points

mp °C	source
91.00	Oxford University MSDS
92.50	PHYSPROP

acetaldehyde C2H4O[2, 3, 61, 64]

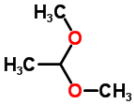
Compound Data

Melting point	**-125.09 °C**	**148.06 K**			
CSID	172	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	44.0526	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.75 g/cm^3
SMILES	CC=O				
STD InChIKey	IKHGUXGNUITLKF-UHFFFAOYAB				

Melting Points

mp °C	source
-125.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-128.00	Alfa Aesar
-124.00	Oxford University MSDS
-123.37	PHYSPROP

acetaldehyde dimethyl acetal C4H10O2[3, 64]



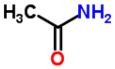
Compound Data

Melting point	**-113.10 °C**	**160.05 K**			
CSID	13854808	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	90.121	**H bond donors**	0	**ACD/LogP**	0.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.84 g/cm^3
SMILES	CC(OC)OC				
STD InChIKey	SPEUIVXLLWOEMJ-UHFFFAOYAV				

Melting Points

mp °C	source
-113.00	Alfa Aesar
-113.20	PHYSPROP

acetamide C2H5NO[2, 3, 61, 64, 64]



Compound Data

Melting point	**80.25 °C**	**353.40 K**			
CSID	173	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	59.0672	**H bond donors**	2	**ACD/LogP**	-1.23
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.95 g/cm^3
SMILES	O=C(N)C				
STD InChIKey	DLFVBJFMPXGRIB-UHFFFAOYAC				

Melting Points

mp °C	source
80.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
79.00	Alfa Aesar
81.00	Oxford University MSDS
81.00	PHYSPROP

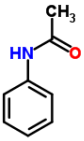
Values not used in calculating the average melting point

-3.80	PHYSPROP[1]

1. Vast majority of literature values support 79-82 - EC

acetanilide C8H9NO[2, 3, 35, 44, 48, 61, 64, 70]

Compound Data



Melting point	**114.37 °C**	**387.52 K**			
CSID	880	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	1	**ACD/LogP**	1.08
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.10 g/cm^3
SMILES	O=C(Nc1ccccc1)C				
STD InChIKey	FZERHIULMFGESH-UHFFFAOYAA				

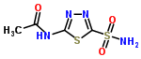
Melting Points

mp °C	source
114.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
115.00	Alfa Aesar
114.30	EPISuite-ChemSpider
114.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
115.00	Oxford University MSDS
114.30	PHYSPROP
114.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
	Values not used in calculating the average melting point
154.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...[1]

1. clearly out of range JCB

acetazolamide C4H6N4O3S2[32, 44, 64]

Compound Data



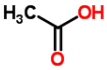
Melting point	**259.83 °C**	**532.98 K**			
CSID	1909	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	222.2454	**H bond donors**	3	**ACD/LogP**	-0.26
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.74 g/cm^3
SMILES	O=S(=O)(c1nnc(s1)NC(=O)C)N				
STD InChIKey	BZKPWHYZMXOIDC-UHFFFAOYAA				

Melting Points

mp °C	source
260.50	DrugBank
258.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
260.50	PHYSPROP

acetic acid C2H4O2[3, 4, 35, 61, 64]

Compound Data



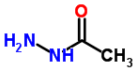
Melting point	**16.78 °C**	**289.93 K**			
CSID	171	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	60.052	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	CC(=O)O				
STD InChIKey	QTBSBXVTEAMEQO-UHFFFAOYAR				

Melting Points

mp °C	source
17.00	Alfa Aesar
17.00	American Petroleum Institute. Research Project 44; Selected ...
16.60	EPISuite-ChemSpider
16.70	Oxford University MSDS
16.60	PHYSPROP

C2H6N2O[3, 64]

acetic hydrazide



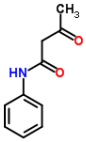
Compound Data

Melting point	**65.50 °C**	**338.65 K**			
CSID	13420	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	74.0818	**H bond donors**	3	**ACD/LogP**	-1.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	O=C(NN)C				
STD InChIKey	OFLXLNCGODUUOT-UHFFFAOYAS				

Melting Points

mp °C	source
64.00	Alfa Aesar
67.00	PHYSPROP

acetoacetanilide C10H11NO2[3, 61, 64]



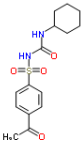
Compound Data

Melting point	**85.67 °C**	**358.82 K**			
CSID	7311	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	177.1998	**H bond donors**	1	**ACD/LogP**	0.85
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	O=C(Nc1ccccc1)CC(=O)C				
STD InChIKey	DYRDKSSFIWVSNM-UHFFFAOYAR				

Melting Points

mp °C	source
85.00	Alfa Aesar
86.00	Oxford University MSDS
86.00	PHYSPROP

acetohexamide C15H20N2O4S[9, 32]



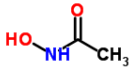
Compound Data

Melting point	**188.50 °C**	**461.65 K**			
CSID	1912	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	324.3953	**H bond donors**	2	**ACD/LogP**	2.44
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.30 g/cm^3
SMILES	O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(C(=O)C)cc2				
STD InChIKey	VGZSUPCWNCWDAN-UHFFFAOYAN				

Melting Points

mp °C	source
188.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
189.00	DrugBank

acetohydroxamic acid C2H5NO2[3, 64]



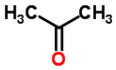
Compound Data

Melting point	**89.25 °C**	**362.40 K**			
CSID	1913	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	75.0666	**H bond donors**	2	**ACD/LogP**	-1.59
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	O=C(NO)C				
STD InChIKey	RRUDCFGSUDOHDG-UHFFFAOYAW				

Melting Points

mp °C	source
88.00	Alfa Aesar
90.50	PHYSPROP

acetone C3H6O[3, 4, 64]



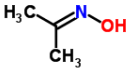
Compound Data

Melting point	**-94.60 °C**	**178.55 K**			
CSID	175	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	58.0791	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3
SMILES	CC(=O)C				
STD InChIKey	CSCPPACGZOOCGX-UHFFFAOYAF				

Melting Points

mp °C	source
-94.00	Alfa Aesar
-95.00	American Petroleum Institute. Research Project 44; Selected ...
-94.80	PHYSPROP

acetone oxime C3H7NO[3, 64]



Compound Data

Melting point	**61.50 °C**	**334.65 K**			
CSID	60524	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	73.0938	**H bond donors**	1	**ACD/LogP**	0.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.91 g/cm^3
SMILES	N(/O)=C(/C)C				
STD InChIKey	PXAJQJMDEXJWFB-UHFFFAOYAK				

Melting Points

mp °C	source
62.00	Alfa Aesar
61.00	PHYSPROP

acetonitrile C2H3N[3, 3, 19, 31, 61, 64, 72, 81, 84]

Compound Data

Melting point	**-46.48 °C**	**226.67 K**			
CSID	6102	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	41.0519	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.75 g/cm^3
SMILES	CC#N				
STD InChIKey	WEVYAHXRMPXWCK-UHFFFAOYAJ				

Melting Points

mp °C	source
-47.00	Alfa Aesar
-46.50	Alfa Aesar
-48.00	Chemical Book
-46.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-46.00	Oxford University MSDS
-43.80	PHYSPROP
-48.00	Sigma-Aldrich
-45.00	Wikipedia
-48.00	Wolfram Alpha

acetyl chloride C2H3ClO[2, 3, 61, 64]

Compound Data

Melting point	**-112.20 °C**	**160.95 K**			
CSID	6127	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	78.4976	**H bond donors**	0	**ACD/LogP**	0.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.12 g/cm^3
SMILES	ClC(=O)C				
STD InChIKey	WETWJCDKMRHUPV-UHFFFAOYAQ				

Melting Points

mp °C	source
-112.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-112.00	Alfa Aesar
-112.00	Oxford University MSDS
-112.80	PHYSPROP

acetylene C2H2[61, 64]

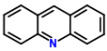
Compound Data

Melting point	**-80.75 °C**	**192.40 K**			
CSID	6086	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	26.0373	**H bond donors**	0	**ACD/LogP**	0.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.57 g/cm^3
SMILES	C#C				
STD InChIKey	HSFWRNGVRCDJHI-UHFFFAOYAY				

Melting Points

mp °C	source
-80.80	Oxford University MSDS
-80.70	PHYSPROP

acridine C13H9N[3, 64]



Compound Data

Melting point	**108.50 °C**	**381.65 K**			
CSID	8860	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	179.2173	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1ccc2c(c1)cc3ccccc3n2				
STD InChIKey	DZBUGLKDJFMEHC-UHFFFAOYAF				

Melting Points

mp °C	source
109.00	Alfa Aesar
108.00	PHYSPROP

acrylaldehyde C3H4O[2, 3, 61, 64]

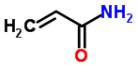
Compound Data

Melting point	**-87.17 °C**	**185.97 K**			
CSID	7559	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	56.0633	**H bond donors**	0	**ACD/LogP**	0.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.80 g/cm^3
SMILES	C=CC=O				
STD InChIKey	HGINCPLSRVDWNT-UHFFFAOYAQ				

Melting Points

mp °C	source
-87.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-87.00	Alfa Aesar
-87.00	Oxford University MSDS
-87.70	PHYSPROP

acrylamide C3H5NO[2, 3, 64]



Compound Data

Melting point	**84.17 °C**	**357.32 K**			
CSID	6331	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	71.0779	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.96 g/cm^3
SMILES	C=CC(=O)N				

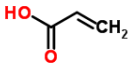
STD InChIKey	HRPVXLWXLXDGHG-UHFFFAOYAS

Melting Points

mp °C	source
84.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
84.00	Alfa Aesar
84.50	PHYSPROP

acrylic acid C3H4O2[2, 3, 32, 64]

Compound Data



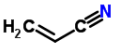
Melting point	**13.00 °C**	**286.15 K**			
CSID	6333	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	72.0627	**H bond donors**	1	**ACD/LogP**	0.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.06 g/cm^3
SMILES	C=CC(=O)O				
STD InChIKey	NIXOWILDQLNWCW-UHFFFAOYAJ				

Melting Points

mp °C	source
13.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
13.00	Alfa Aesar
13.50	DrugBank
12.50	PHYSPROP

acrylonitrile C3H3N[3, 64]

Compound Data



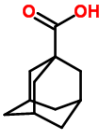
Melting point	**-83.75 °C**	**189.40 K**			
CSID	7567	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	53.0626	**H bond donors**	0	**ACD/LogP**	0.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.80 g/cm^3
SMILES	C=CC#N				
STD InChIKey	NLHHRLWOUZZQLW-UHFFFAOYAG				

Melting Points

mp °C	source
-84.00	Alfa Aesar
-83.50	PHYSPROP

adamantane-1-carboxylic acid C11H16O2[3, 64]

Compound Data



Melting point	**174.75 °C**	**447.90 K**			
CSID	12680	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	180.2435	**H bond donors**	1	**ACD/LogP**	2.59
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	C1C2CC3CC1CC(C2)(C3)C(=O)O				
STD InChIKey	JIMXXGFJRDUSRO-UHFFFAOYAT				

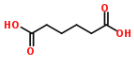
Melting Points

mp °C	source
175.00	Alfa Aesar
174.50	PHYSPROP

adipic acid C6H10O4[2, 3, 61, 64]

Compound Data

Melting point	**152.80 °C**	**425.95 K**			
CSID	191	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	146.1412	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.25 g/cm^3



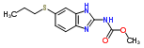
SMILES	C(CCC(=O)O)CC(=O)O
STD InChIKey	WNLRTRBMVRJNCN-UHFFFAOYAY

Melting Points

mp °C	source
153.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
153.00	Alfa Aesar
152.00	Oxford University MSDS
153.20	PHYSPROP

albendazole C12H15N3O2S[3, 9, 32, 48, 64]

Compound Data



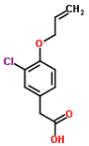
Melting point	**208.60 °C**	**481.75 K**			
CSID	1998	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	265.3314	**H bond donors**	2	**ACD/LogP**	3.07
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.30 g/cm^3
SMILES	O=C(OC)Nc2nc1ccc(SCCC)cc1n2				
STD InChIKey	HXHWSAZORRCQMX-UHFFFAOYAA				

Melting Points

mp °C	source
209.00	Alfa Aesar
208.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
209.00	DrugBank
208.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
209.00	PHYSPROP

alclofenac C11H11ClO3[9, 44, 48, 64]

Compound Data



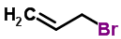
Melting point	**92.25 °C**	**365.40 K**			
CSID	28714	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.6562	**H bond donors**	1	**ACD/LogP**	2.77
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.25 g/cm^3
SMILES	Clc1cc(ccc1OC\C=C)CC(=O)O				
STD InChIKey	ARHWPKZXBHOEEE-UHFFFAOYAY				

Melting Points

mp °C	source
92.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
92.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
92.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
92.50	PHYSPROP

allyl bromide C3H5Br[3, 59, 59, 64]

Compound Data



Melting point	**-119.10 °C**	**154.05 K**			
CSID	7553	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.9758	**H bond donors**	0	**ACD/LogP**	1.79
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	C=CCBr				
STD InChIKey	BHELZAPQIKSEDF-UHFFFAOYAI				

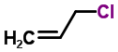
Melting Points

mp °C	source
-119.00	Alfa Aesar

-119.00	NIST Web Book
-119.40	NIST Web Book
-119.00	PHYSPROP
	Values not used in calculating the average melting point
-50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...[1]

1. error from secondary database copying from SA JCB

allyl chloride C3H5Cl[3, 31, 61, 64]



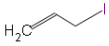
Compound Data

Melting point	**-134.62 °C**	**138.52 K**			
CSID	13836674	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	76.5248	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.91 g/cm^3
SMILES	C=CCCl				
STD InChIKey	OSDWBNJEKMUWAV-UHFFFAOYAQ				

Melting Points

mp °C	source
-135.00	Alfa Aesar
-135.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-134.00	Oxford University MSDS
-134.50	PHYSPROP

allyl iodide C3H5I[3, 31, 64]



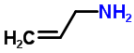
Compound Data

Melting point	**-99.10 °C**	**174.05 K**			
CSID	21171407	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	167.9763	**H bond donors**	0	**ACD/LogP**	2.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.83 g/cm^3
SMILES	C=CCI				
STD InChIKey	HFEHLDPGIKPNKL-UHFFFAOYAC				

Melting Points

mp °C	source
-99.00	Alfa Aesar
-99.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-99.30	PHYSPROP

allylamine C3H7N[2, 3, 64]



Compound Data

Melting point	**-88.07 °C**	**185.08 K**			
CSID	13835977	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	57.0944	**H bond donors**	2	**ACD/LogP**	0.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.74 g/cm^3
SMILES	C=CCN				
STD InChIKey	VVJKKWFAADXIJK-UHFFFAOYAW				

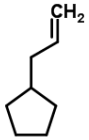
Melting Points

mp °C	source
-88.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-88.00	Alfa Aesar
-88.20	PHYSPROP

allylcyclopentane C8H14[3, 64]

Compound Data

Melting point	**-110.85 °C**	**162.30 K**			
CSID	69505	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	110.1968	**H bond donors**	0	**ACD/LogP**	3.87



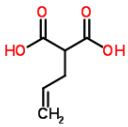
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.80 g/cm^3
SMILES	C=C\CC1CCCC1				
STD InChIKey	NHIDGVQVYHCGEK-UHFFFAOYAF				

Melting Points

mp °C	source
-111.00	Alfa Aesar
-110.70	PHYSPROP

allylmalonic acid C6H8O4[3, 64]

Compound Data



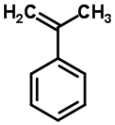
Melting point	**104.50 °C**	**377.65 K**			
CSID	68265	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	144.1253	**H bond donors**	2	**ACD/LogP**	0.73
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.28 g/cm^3
SMILES	O=C(O)C(C(=O)O)C\C=C				
STD InChIKey	ZDZVKPXKLLLOOA-UHFFFAOYAQ				

Melting Points

mp °C	source
104.00	Alfa Aesar
105.00	PHYSPROP

alpha-methylstyrene C9H10[3, 4, 64]

Compound Data



Melting point	**-23.07 °C**	**250.08 K**			
CSID	7129	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.1757	**H bond donors**	0	**ACD/LogP**	3.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	CC(=C)c1ccccc1				
STD InChIKey	XYLMUPLGERFSHI-UHFFFAOYAS				

Melting Points

mp °C	source
-23.00	Alfa Aesar
-23.00	American Petroleum Institute. Research Project 44; Selected ...
-23.20	PHYSPROP

alphenal C13H12N2O3[9, 44, 48, 64]

Compound Data

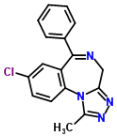
Melting point	**156.75 °C**	**429.90 K**			
CSID	7975	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	244.246	**H bond donors**	2	**ACD/LogP**	1.69
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(c2ccccc2)C\C=C				
STD InChIKey	WOIGZSBYKGQJGL-UHFFFAOYAF				

Melting Points

mp °C	source
156.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
158.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
156.50	PHYSPROP

alprazolam C17H13ClN4[32, 44]

Compound Data



Melting point	**229.12 °C**	**502.27 K**			
CSID	2034	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	308.7649	**H bond donors**	0	**ACD/LogP**	1.92
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	Cc1nnc2n1-c3ccc(cc3C(=NC2)c4ccccc4)Cl				
STD InChIKey	VREFGVBLTWBCJP-UHFFFAOYAT				

Melting Points

mp °C	source
228.25	DrugBank
230.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...

amiloride C6H8ClN7O[32, 64]

Compound Data

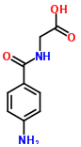
Melting point	**240.50 °C**	**513.65 K**			
CSID	15403	**H bond acceptors**	8	**Rule of 5 violations**	1
Molecular weight	229.627	**H bond donors**	8	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.11 g/cm^3
SMILES	Clc1nc(C(=O)\N=C(/N)N)c(nc1N)N				
STD InChIKey	XSDQTOBWRPYKKA-UHFFFAOYAR				

Melting Points

mp °C	source
240.00	DrugBank
241.00	PHYSPROP

aminohippuric acid C9H10N2O3[32, 64]

Compound Data



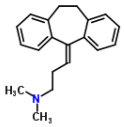
Melting point	**199.00 °C**	**472.15 K**			
CSID	2063	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	194.1873	**H bond donors**	4	**ACD/LogP**	-0.58
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.36 g/cm^3
SMILES	O=C(c1ccc(N)cc1)NCC(=O)O				
STD InChIKey	HSMNQINEKMPTIC-UHFFFAOYAW				

Melting Points

mp °C	source
199.50	DrugBank
198.50	PHYSPROP

amitriptyline C20H23N[32, 44, 64]

Compound Data



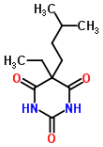
Melting point	**196.33 °C**	**469.48 K**			
CSID	2075	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	277.4033	**H bond donors**	0	**ACD/LogP**	4.92
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	c3cc2c(/C(c1c(cccc1)CC2)=C\CCN(C)C)cc3				
STD InChIKey	KRMDCWKBEZIMAB-UHFFFAOYAI				

Melting Points

mp °C	source
196.50	DrugBank
196.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
196.50	PHYSPROP

amobarbital C11H18N2O3[9, 35, 44, 48, 64]

Compound Data



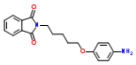
Melting point	**156.60 °C**	**429.75 K**			
CSID	2079	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	226.2722	**H bond donors**	2	**ACD/LogP**	2.05
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.07 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(CCC(C)C)CC				
STD InChIKey	VIROVYVQCGLCII-UHFFFAOYAO				

Melting Points

mp °C	source
156.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
157.00	EPISuite-ChemSpider
157.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
157.00	PHYSPROP

amphotalide C19H20N2O3[9, 48, 64]

Compound Data



Melting point	**113.17 °C**	**386.32 K**			
CSID	64830	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	324.3737	**H bond donors**	2	**ACD/LogP**	3.14
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.25 g/cm^3
SMILES	O=C2c1ccccc1C(=O)N2CCCCCOc3ccc(N)cc3				
STD InChIKey	GIIGAFADHXYOPM-UHFFFAOYAI				

Melting Points

mp °C	source
113.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
113.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
113.50	PHYSPROP

ampyrone C11H13N3O[3, 61, 64]

Compound Data

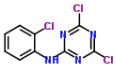
Melting point	**108.00 °C**	**381.15 K**			
CSID	2066	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	203.2404	**H bond donors**	2	**ACD/LogP**	-0.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	O=C2\C(=C(/N(N2c1ccccc1)C)C)N				
STD InChIKey	RLFWWDJHLFCNIJ-UHFFFAOYAT				

Melting Points

mp °C	source
108.00	Alfa Aesar
107.00	Oxford University MSDS
109.00	PHYSPROP

anilazine C9H5Cl3N4[61, 64]

Compound Data



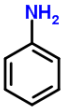
Melting point	**159.75 °C**	**432.90 K**			
CSID	7260	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	275.5218	**H bond donors**	1	**ACD/LogP**	3.07
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.61 g/cm^3
SMILES	Clc1nc(nc(Cl)n1)Nc2ccccc2Cl				
STD InChIKey	IMHBYKMAHXWHRP-UHFFFAOYAQ				

Melting Points

mp °C	source
159.50	Oxford University MSDS
160.00	PHYSPROP

aniline C6H7N[3, 18, 20, 31, 35, 46, 61, 61, 64, 81]

Compound Data



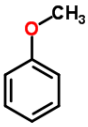
Melting point	**-6.07 °C**	**267.08 K**			
CSID	5889	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	93.1265	**H bond donors**	2	**ACD/LogP**	1.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	c1ccc(cc1)N				
STD InChIKey	PAYRUJLWNCNPSJ-UHFFFAOYAP				

Melting Points

mp °C	source
-6.00	Alfa Aesar
-6.20	ChemGuide
-6.00	Chemical Land
-6.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-6.00	EPISuite-ChemSpider
-6.20	Internet Encyclopedia of Science
-6.00	Oxford University MSDS
-6.00	Oxford University MSDS
-6.02	PHYSPROP
-6.30	Wikipedia

anisole C7H8O[2, 3, 61, 64]

Compound Data



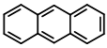
Melting point	**-37.12 °C**	**236.02 K**			
CSID	7238	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	108.1378	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.95 g/cm^3
SMILES	COc1ccccc1				
STD InChIKey	RDOXTESZEPMUJZ-UHFFFAOYAP				

Melting Points

mp °C	source
-37.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-37.00	Alfa Aesar
-37.00	Oxford University MSDS
-37.50	PHYSPROP

anthracene C14H10[2, 3, 44, 64, 70, 70]

Compound Data



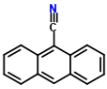
Melting point	**216.17 °C**	**489.32 K**			
CSID	8111	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	178.2292	**H bond donors**	0	**ACD/LogP**	4.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	c1ccc2cc3ccccc3cc2c1				
STD InChIKey	MWPLVEDNUUSJAV-UHFFFAOYAK				

Melting Points

mp °C	source
216.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
216.00	Alfa Aesar
218.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
215.00	PHYSPROP
216.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
216.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

anthracene-9-carbonitrile C15H9N[3, 61, 64]

Compound Data



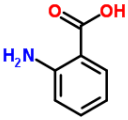
Melting point	**175.67 °C**	**448.82 K**			
CSID	13924	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	203.2387	**H bond donors**	0	**ACD/LogP**	4.12
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	N#Cc2c3c(cc1c2cccc1)cccc3				
STD InChIKey	KEQZHLAEKAVZLY-UHFFFAOYAB				

Melting Points

mp °C	source
177.00	Alfa Aesar
175.00	Oxford University MSDS
175.00	PHYSPROP

anthranilic acid C7H7NO2[2, 3, 64]

Compound Data



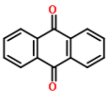
Melting point	**146.00 °C**	**419.15 K**			
CSID	222	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	3	**ACD/LogP**	1.27
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	c1ccc(c(c1)C(=O)O)N				
STD InChIKey	RWZYAGGXGHYGMB-UHFFFAOYAS				

Melting Points

mp °C	source
146.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
147.00	Alfa Aesar
145.00	PHYSPROP

anthraquinone C14H8O2[2, 3, 64]

Compound Data



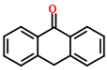
Melting point	**285.00 °C**	**558.15 K**			
CSID	13835294	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	208.2121	**H bond donors**	0	**ACD/LogP**	3.06
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.31 g/cm^3
SMILES	c1ccc2c(c1)C(=O)c3ccccc3C2=O				
STD InChIKey	RZVHIXYEVGDQDX-UHFFFAOYAA				

Melting Points

mp °C	source
284.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
285.00	Alfa Aesar
286.00	PHYSPROP

anthrone C14H10O[3, 61, 64]

Compound Data



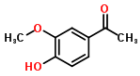
Melting point	**156.17 °C**	**429.32 K**			
CSID	6751	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	194.2286	**H bond donors**	0	**ACD/LogP**	3.58
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	O=C2c1c(cccc1)Cc3c2cccc3				
STD InChIKey	RJGDLRCDCYRQOQ-UHFFFAOYAA				

Melting Points

mp °C	source
157.00	Alfa Aesar
156.50	Oxford University MSDS
155.00	PHYSPROP

apocynin C9H10O3[3, 3, 64]

Compound Data



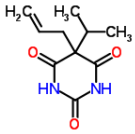
Melting point	**114.50 °C**	**387.65 K**			
CSID	21106900	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	1.39
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	Oc1ccc(cc1OC)C(C)=O				
STD InChIKey	DFYRUELUNQRZTB-UHFFFAOYAW				

Melting Points

mp °C	source
114.50	Alfa Aesar
114.00	Alfa Aesar
115.00	PHYSPROP

aprobarbital C10H14N2O3[32, 44, 64]

Compound Data



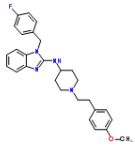
Melting point	**141.57 °C**	**414.72 K**			
CSID	6221	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	210.2298	**H bond donors**	2	**ACD/LogP**	1.11
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.12 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(C(C)C)C\C=C				
STD InChIKey	UORJNBVJVRLXMQ-UHFFFAOYAV				

Melting Points

mp °C	source
141.00	DrugBank
142.70	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
141.00	PHYSPROP

astemizole C28H31FN4O[9, 32, 48, 64]

Compound Data



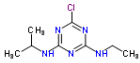
Melting point	**149.05 °C**	**422.20 K**			
CSID	2160	**H bond acceptors**	5	**Rule of 5 violations**	1
Molecular weight	458.5703	**H bond donors**	1	**ACD/LogP**	5.80
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.20 g/cm^3
SMILES	Fc1ccc(cc1)Cn2c5ccccc5nc2NC4CCN(CCc3ccc(OC)cc3)CC4				
STD InChIKey	GXDALQBWZGODGZ-UHFFFAOYAC				

Melting Points

mp °C	source
149.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
149.10	DrugBank
149.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
149.10	PHYSPROP

atrazine C8H14ClN5[44, 64, 70]

Compound Data

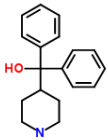


Melting point	**173.50 °C**	**446.65 K**			
CSID	2169	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	215.6833	**H bond donors**	2	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	Clc1nc(nc(n1)NC(C)C)NCC				
STD InChIKey	MXWJVTOOROXGIU-UHFFFAOYAJ				

Melting Points

mp °C	source
172.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
173.00	PHYSPROP
175.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

azacyclonol C18H21NO[9, 48, 64]



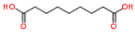
Compound Data

Melting point	**160.17 °C**	**433.32 K**			
CSID	14952	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	267.3654	**H bond donors**	2	**ACD/LogP**	3.25
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.10 g/cm^3
SMILES	OC(c1ccccc1)(c2ccccc2)C3CCNCC3				
STD InChIKey	ZMISODWVFHHWNR-UHFFFAOYAZ				

Melting Points

mp °C	source
160.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
160.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
160.50	PHYSPROP

azelaic acid C9H16O4[3, 32, 64]



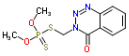
Compound Data

Melting point	**105.00 °C**	**378.15 K**			
CSID	2179	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	188.2209	**H bond donors**	2	**ACD/LogP**	1.33
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.13 g/cm^3
SMILES	O=C(O)CCCCCCCC(=O)O				
STD InChIKey	BDJRBEYXGGNYIS-UHFFFAOYAK				

Melting Points

mp °C	source
102.00	Alfa Aesar
106.50	DrugBank
106.50	PHYSPROP

azinphos-methyl C10H12N3O3PS2[61, 64]



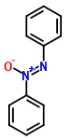
Compound Data

Melting point	**72.50 °C**	**345.65 K**			
CSID	2181	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	317.3243	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.51 g/cm^3
SMILES	S=P(OC)(OC)SCN1\N=N/c2ccccc2C1=O				
STD InChIKey	CJJOSEISRRTUQB-UHFFFAOYAL				

Melting Points

mp °C	source
72.00	Oxford University MSDS
73.00	PHYSPROP

azoxybenzene C12H10N2O[3, 64]



Compound Data

Melting point	**35.50 °C**	**308.65 K**			
CSID	9894	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	198.2206	**H bond donors**	0	**ACD/LogP**	4.09
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	[O-]\[N+](=N/c1ccccc1)c2ccccc2				
STD InChIKey	GAUZCKBSTZFWCT-YPKPFQOOBT				

Melting Points

mp °C	source
35.00	Alfa Aesar
36.00	PHYSPROP

azulene C10H8[3, 61, 64]

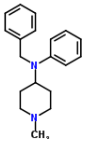
Compound Data

Melting point	**99.50 °C**	**372.65 K**			
CSID	8876	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	128.1705	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.04 g/cm^3
SMILES	c1cccc2cccc2c1				
STD InChIKey	CUFNKYGDVFVPHO-UHFFFAOYAT				

Melting Points

mp °C	source
100.00	Alfa Aesar
99.50	Oxford University MSDS
99.00	PHYSPROP

bamipine C19H24N2[9, 48, 64]



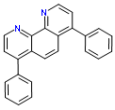
Compound Data

Melting point	**114.33 °C**	**387.48 K**			
CSID	65061	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	280.4073	**H bond donors**	0	**ACD/LogP**	4.60
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.07 g/cm^3
SMILES	N(c1ccccc1)(Cc2ccccc2)C3CCN(C)CC3				
STD InChIKey	VZSXTYKGYWISGQ-UHFFFAOYAD				

Melting Points

mp °C	source
114.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
114.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
115.00	PHYSPROP

bathophenanthroline C24H16N2[3, 61]



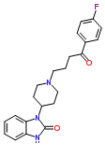
Compound Data

Melting point	**219.00 °C**	**492.15 K**			
CSID	65648	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	332.3972	**H bond donors**	0	**ACD/LogP**	6.16
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	c1ccc(cc1)c2ccnc3c2ccc4c3nccc4c5ccccc5				
STD InChIKey	DHDHJYNTEFLIHY-UHFFFAOYAP				

Melting Points

mp °C	source
220.00	Alfa Aesar
218.00	Oxford University MSDS

benperidol C22H24FN3O2[9, 44, 48, 64]



Compound Data

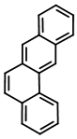
Melting point	**170.45 °C**	**443.60 K**			
CSID	15521	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	381.4433	**H bond donors**	1	**ACD/LogP**	4.09
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.24 g/cm^3
SMILES	Fc1ccc(cc1)C(=O)CCCN4CCC(N3c2ccccc2NC3=O)CC4				
STD InChIKey	FEBOTPHFXYHVPL-UHFFFAOYAW				

Melting Points

mp °C	source
170.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
170.90	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...

170.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
170.90	PHYSPROP

benz(a)anthracene C18H12[44, 61, 64]



Compound Data

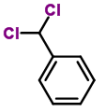
Melting point	**159.00 °C**	**432.15 K**			
CSID	5739	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	228.2879	**H bond donors**	0	**ACD/LogP**	5.73
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1ccc2c(c1)ccc3c2cc4ccccc4c3				
STD InChIKey	DXBHBZVCASKNBY-UHFFFAOYAM				

Melting Points

mp °C	source
160.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
158.00	Oxford University MSDS
	Values not used in calculating the average melting point
84.00	PHYSPROP[1]

1. All other sources support 156-162 - EC

benzal chloride C7H6Cl2[2, 3, 64]



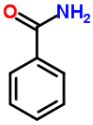
Compound Data

Melting point	**-16.33 °C**	**256.82 K**			
CSID	13882337	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	161.0285	**H bond donors**	0	**ACD/LogP**	2.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	ClC(Cl)c1ccccc1				
STD InChIKey	CAHQGWAXKLQREW-UHFFFAOYAD				

Melting Points

mp °C	source
-16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-16.00	Alfa Aesar
-17.00	PHYSPROP

benzamide C7H7NO[2, 3, 44, 61, 64, 72]



Compound Data

Melting point	**128.10 °C**	**401.25 K**			
CSID	2241	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	121.1366	**H bond donors**	2	**ACD/LogP**	0.75
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	c1ccc(cc1)C(=O)N				
STD InChIKey	KXDAEFPNCMNJSK-UHFFFAOYAA				

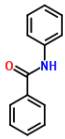
Melting Points

mp °C	source
129.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
127.00	Alfa Aesar
130.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
127.00	Oxford University MSDS
129.10	PHYSPROP
126.50	Sigma-Aldrich

benzanilide C13H11NO[2, 3, 64]

Compound Data

Melting point	**163.33 °C**	**436.48 K**			
CSID	6900	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	197.2325	**H bond donors**	1	**ACD/LogP**	2.46



Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	c1ccc(cc1)C(=O)Nc2ccccc2				
STD InChIKey	ZVSKZLHKADLHSD-UHFFFAOYAY				

Melting Points

mp °C	source
163.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
164.00	Alfa Aesar
163.00	PHYSPROP

benzene C6H6[3, 3, 4, 28, 34, 58, 61, 64, 81]

Compound Data

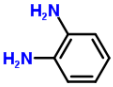
Melting point	**5.51 °C**	**278.66 K**			
CSID	236	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	78.1118	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1ccccc1				
STD InChIKey	UHOVQNZJYSORNB-UHFFFAOYAH				

Melting Points

mp °C	source
5.51	Alfa Aesar
5.00	Alfa Aesar
6.00	American Petroleum Institute. Research Project 44; Selected ...
5.49	CRC Handbook of Chemistry and Physics
5.50	EPA
5.60	NIOSH
5.50	Oxford University MSDS
5.50	PHYSPROP
5.50	Wikipedia

benzene-1,2-diamine C6H8N2[2, 3, 61, 64]

Compound Data



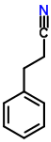
Melting point	**101.75 °C**	**374.90 K**			
CSID	13837582	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	4	**ACD/LogP**	0.05
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	Nc1ccccc1N				
STD InChIKey	GEYOCULIXLDCMW-UHFFFAOYAR				

Melting Points

mp °C	source
101.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
102.00	Alfa Aesar
101.50	Oxford University MSDS
102.50	PHYSPROP

benzenepropanenitrile C9H9N[2, 3, 64]

Compound Data



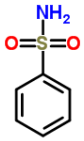
Melting point	**-1.67 °C**	**271.48 K**			
CSID	12061	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	131.1745	**H bond donors**	0	**ACD/LogP**	1.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	N#CCCc1ccccc1				
STD InChIKey	ACRWYXSKEHUQDB-UHFFFAOYAW				

Melting Points

mp °C	source
-2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-2.00	Alfa Aesar
-1.00	PHYSPROP

benzenesulfonamide C6H7NO2S[2, 3, 64]

Compound Data



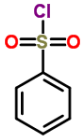
Melting point	**151.67 °C**	**424.82 K**			
CSID	7092	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	157.1903	**H bond donors**	2	**ACD/LogP**	0.33
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	O=S(=O)(N)c1ccccc1				
STD InChIKey	KHBQMWCZKVMBLN-UHFFFAOYAA				

Melting Points

mp °C	source
151.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
153.00	Alfa Aesar
151.00	PHYSPROP

benzenesulfonyl chloride C6H5ClO2S[3, 61, 64]

Compound Data



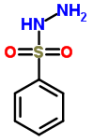
Melting point	**14.83 °C**	**287.98 K**			
CSID	7091	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	176.6207	**H bond donors**	0	**ACD/LogP**	1.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	O=S(=O)(Cl)c1ccccc1				
STD InChIKey	CSKNSYBAZOQPLR-UHFFFAOYAR				

Melting Points

mp °C	source
15.00	Alfa Aesar
15.00	Oxford University MSDS
14.50	PHYSPROP

benzenesulfonyl hydrazide C6H8N2O2S[3, 64]

Compound Data



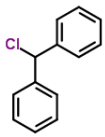
Melting point	**102.50 °C**	**375.65 K**			
CSID	59146	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.2049	**H bond donors**	3	**ACD/LogP**	-0.14
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.35 g/cm^3
SMILES	O=S(=O)(NN)c1ccccc1				
STD InChIKey	VJRITMATACIYAF-UHFFFAOYAH				

Melting Points

mp °C	source
103.00	Alfa Aesar
102.00	PHYSPROP

benzhydryl chloride C13H11Cl[2, 3, 64]

Compound Data



Melting point	**17.00 °C**	**290.15 K**			
CSID	6768	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	202.6794	**H bond donors**	0	**ACD/LogP**	3.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.12 g/cm^3
SMILES	ClC(c1ccccc1)c2ccccc2				

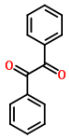
STD InChIKey	ZDVDCDLBOLSVGM-UHFFFAOYAO

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
19.00	Alfa Aesar
16.00	PHYSPROP

benzil C14H10O2[2, 3, 61, 64, 70]

Compound Data



Melting point	**94.86 °C**	**368.01 K**			
CSID	8329	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	210.228	**H bond donors**	0	**ACD/LogP**	3.38
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	c1ccc(cc1)C(=O)C(=O)c2ccccc2				
STD InChIKey	WURBFLDFSFBTLW-UHFFFAOYAZ				

Melting Points

mp °C	source
95.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
95.00	Alfa Aesar
94.50	Oxford University MSDS
94.80	PHYSPROP
95.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

benzimidazole C7H6N2[3, 35, 61, 64]

Compound Data

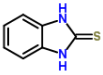
Melting point	**171.00 °C**	**444.15 K**			
CSID	5593	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1359	**H bond donors**	1	**ACD/LogP**	1.32
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	c1ccc2c(c1)[nH]cn2				
STD InChIKey	HYZJCKYKOHLVJF-UHFFFAOYAX				

Melting Points

mp °C	source
172.00	Alfa Aesar
170.50	EPISuite-ChemSpider
171.00	Oxford University MSDS
170.50	PHYSPROP

benzimidazole-2-thiol C7H6N2S[3, 61, 64]

Compound Data



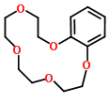
Melting point	**301.33 °C**	**574.48 K**			
CSID	616466	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.2009	**H bond donors**	2	**ACD/LogP**	1.66
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	S=C2Nc1ccccc1N2				
STD InChIKey	YHMYGUUIMTVXNW-UHFFFAOYAG				

Melting Points

mp °C	source
303.00	Alfa Aesar
303.00	Oxford University MSDS
298.00	PHYSPROP

benzo-15-crown-5 C14H20O5[3, 64]

Compound Data



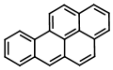
Melting point	**79.50 °C**	**352.65 K**			
CSID	75956	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	268.3056	**H bond donors**	0	**ACD/LogP**	0.65
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	O1c2c(OCCOCCOCCOCC1)cccc2				
STD InChIKey	FNEPSTUXZLEUCK-UHFFFAOYAC				

Melting Points

mp °C	source
80.00	Alfa Aesar
79.00	PHYSPROP

benzo(a)pyrene C20H12[3, 44, 61, 64, 70]

Compound Data



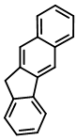
Melting point	**177.90 °C**	**451.05 K**			
CSID	2246	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	252.3093	**H bond donors**	0	**ACD/LogP**	6.19
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	c1ccc2c(c1)cc3ccc4cccc5c4c3c2cc5				
STD InChIKey	FMMWHPNWAFZXNH-UHFFFAOYAQ				

Melting Points

mp °C	source
179.00	Alfa Aesar
179.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
176.00	Oxford University MSDS
176.50	PHYSPROP
179.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

benzo(b)fluorene C17H12[64, 70]

Compound Data



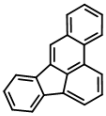
Melting point	**210.00 °C**	**483.15 K**			
CSID	8846	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	216.2772	**H bond donors**	0	**ACD/LogP**	5.39
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1cccc4c1c2c(cc3c(c2)cccc3)C4				
STD InChIKey	HAPOJKSPCGLOOD-UHFFFAOYAL				

Melting Points

mp °C	source
212.00	PHYSPROP
208.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

benzo[b]fluoranthene C20H12[61, 64]

Compound Data

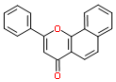


Melting point	**166.00 °C**	**439.15 K**			
CSID	8799	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	252.3093	**H bond donors**	0	**ACD/LogP**	6.19
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	c1ccc2c(c1)cc-3c4c2cccc4-c5c3cccc5				
STD InChIKey	FTOVXSOBNPWTSH-UHFFFAOYAM				

Melting Points

mp °C	source
164.00	Oxford University MSDS
168.00	PHYSPROP

benzo[h]flavone C19H12O2[3, 61]



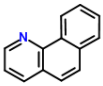
Compound Data

Melting point	**155.50 °C**	**428.65 K**			
CSID	11297	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	272.2974	**H bond donors**	0	**ACD/LogP**	4.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.28 g/cm^3
SMILES	O=C\1c4c(O/C(=C/1)c2ccccc2)c3ccccc3cc4				
STD InChIKey	VFMMPHCGEFXGIP-UHFFFAOYAW				

Melting Points

mp °C	source
158.00	Alfa Aesar
153.00	Oxford University MSDS

benzo[h]quinoline C13H9N[3, 64]



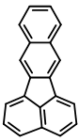
Compound Data

Melting point	**51.00 °C**	**324.15 K**			
CSID	8836	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	179.2173	**H bond donors**	0	**ACD/LogP**	3.31
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	n2cccc3ccc1ccccc1c23				
STD InChIKey	WZJYKHNJTSNBHV-UHFFFAOYAX				

Melting Points

mp °C	source
50.00	Alfa Aesar
52.00	PHYSPROP

benzo[k]fluoranthene C20H12[61, 64]



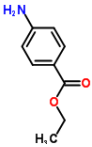
Compound Data

Melting point	**216.50 °C**	**489.65 K**			
CSID	8804	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	252.3093	**H bond donors**	0	**ACD/LogP**	6.19
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	c1ccc2cc-3c(cc2c1)-c4cccc5c4c3ccc5				
STD InChIKey	HAXBIWFMXWRORI-UHFFFAOYAA				

Melting Points

mp °C	source
216.00	Oxford University MSDS
217.00	PHYSPROP

benzocaine C9H11NO2[2, 3, 35, 44, 61, 64, 70]



Compound Data

Melting point	**89.86 °C**	**363.01 K**			
CSID	13854242	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	165.1891	**H bond donors**	2	**ACD/LogP**	1.95
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	O=C(OCC)c1ccc(N)cc1				
STD InChIKey	BLFLLBZGZJTVJG-UHFFFAOYAZ				

Melting Points

mp °C	source
89.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
90.00	Alfa Aesar
92.00	EPISuite-ChemSpider
89.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
88.00	Oxford University MSDS
92.00	PHYSPROP
89.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

benzofuroxan C6H4N2O2[3, 48, 64]

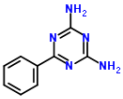
Compound Data

Melting point	**69.33 °C**	**342.48 K**			
CSID	61388	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	136.1082	**H bond donors**	0	**ACD/LogP**	1.43
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	[O-][n+]1onc2ccccc12				
STD InChIKey	OKEAMBAZBICIFP-UHFFFAOYAO				

Melting Points

mp °C	source
69.00	Alfa Aesar
69.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
70.00	PHYSPROP

benzoguanamine C9H9N5[3, 64]



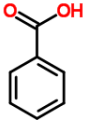
Compound Data

Melting point	**226.75 °C**	**499.90 K**			
CSID	6797	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	187.2013	**H bond donors**	4	**ACD/LogP**	1.36
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	n1c(nc(nc1c2ccccc2)N)N				
STD InChIKey	GZVHEAJQGPRDLQ-UHFFFAOYAJ				

Melting Points

mp °C	source
227.00	Alfa Aesar
226.50	PHYSPROP

benzoic acid C7H6O2[2, 3, 9, 28, 35, 44, 48, 56, 61, 64, 70, 70, 72]



Compound Data

Melting point	**122.38 °C**	**395.53 K**			
CSID	238	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1213	**H bond donors**	1	**ACD/LogP**	1.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.20 g/cm^3
SMILES	c1ccc(cc1)C(=O)O				
STD InChIKey	WPYMKLBDIGXBTP-UHFFFAOYAD				

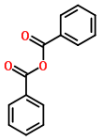
Melting Points

mp °C	source
123.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
123.00	Alfa Aesar
122.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
122.35	CRC Handbook of Chemistry and Physics
122.40	EPISuite-ChemSpider
122.40	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
122.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
122.40	Merck Index
122.00	Oxford University MSDS
122.40	PHYSPROP
122.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
122.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
123.00	Sigma-Aldrich

benzoic anhydride C14H10O3[3, 64]

Compound Data

Melting point	**42.25 °C**	**315.40 K**



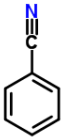
CSID	6899	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.2274	**H bond donors**	0	**ACD/LogP**	3.02
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.21 g/cm^3
SMILES	O=C(OC(=O)c1ccccc1)c2ccccc2				
STD InChIKey	CHIHQLCVLOXUJW-UHFFFAOYAU				

Melting Points

mp °C	source
42.00	Alfa Aesar
42.50	PHYSPROP

benzonitrile C7H5N[2, 3, 61, 64]

Compound Data



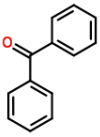
Melting point	**-12.93 °C**	**260.22 K**			
CSID	7224	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	103.1213	**H bond donors**	0	**ACD/LogP**	1.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.03 g/cm^3
SMILES	c1ccc(cc1)C#N				
STD InChIKey	JFDZBHWFFUWGJE-UHFFFAOYAY				

Melting Points

mp °C	source
-13.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-13.00	Alfa Aesar
-13.00	Oxford University MSDS
-12.70	PHYSPROP

benzophenone C13H10O[3, 31, 32, 61, 64]

Compound Data



Melting point	**48.28 °C**	**321.43 K**			
CSID	2991	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.2179	**H bond donors**	0	**ACD/LogP**	3.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	O=C(c1ccccc1)c2ccccc2				
STD InChIKey	RWCCWEUUXYIKHB-UHFFFAOYAX				

Melting Points

mp °C	source
49.00	Alfa Aesar
48.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
47.90	DrugBank
48.00	Oxford University MSDS
48.50	PHYSPROP

benzoquinone C6H4O2[2, 3, 61, 64]

Compound Data

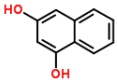
Melting point	**114.42 °C**	**387.57 K**			
CSID	4489	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.0948	**H bond donors**	0	**ACD/LogP**	0.39
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	C1=CC(=O)C=CC1=O				
STD InChIKey	AZQWKYJCGOJGHM-UHFFFAOYAR				

Melting Points

mp °C	source
114.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
114.00	Alfa Aesar
114.00	Oxford University MSDS

115.70	PHYSPROP

benzoresorcinol C10H8O2[3, 64]



Compound Data

Melting point	**124.25 °C**	**397.40 K**			
CSID	8282	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.1693	**H bond donors**	2	**ACD/LogP**	1.99
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	Oc2c1c(cccc1)cc(O)c2				
STD InChIKey	XOOMNEFVDUTJPP-UHFFFAOYAY				

Melting Points

mp °C	source
125.00	Alfa Aesar
123.50	PHYSPROP

benzothiophene C8H6S[3, 64, 64]

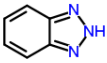
Compound Data

Melting point	**31.17 °C**	**304.32 K**			
CSID	6951	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.1982	**H bond donors**	0	**ACD/LogP**	4.38
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	s2c1ccccc1cc2				
STD InChIKey	FCEHBMOGCRZNNI-UHFFFAOYAI				

Melting Points

mp °C	source
30.00	Alfa Aesar
32.00	PHYSPROP
31.50	PHYSPROP

benzotriazole C6H5N3[3, 61, 64]



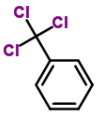
Compound Data

Melting point	**98.33 °C**	**371.48 K**			
CSID	6950	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	119.124	**H bond donors**	1	**ACD/LogP**	1.14
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.35 g/cm^3
SMILES	n1c2ccccc2nn1				
STD InChIKey	QRUDEWIWKLJBPS-UHFFFAOYAH				

Melting Points

mp °C	source
98.00	Alfa Aesar
97.00	Oxford University MSDS
100.00	PHYSPROP

benzotrichloride C7H5Cl3[2, 3, 61, 64]



Compound Data

Melting point	**-5.50 °C**	**267.65 K**			
CSID	13882366	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	195.4736	**H bond donors**	0	**ACD/LogP**	3.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	ClC(Cl)(Cl)c1ccccc1				
STD InChIKey	XEMRAKSQROQPBR-UHFFFAOYAF				

Melting Points

mp °C	source
-8.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

-4.00	Alfa Aesar
-5.00	Oxford University MSDS
-5.00	PHYSPROP

benzoxazole C7H5NO[3, 64]

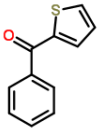
Compound Data

Melting point	**30.50 °C**	**303.65 K**			
CSID	8873	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	119.1207	**H bond donors**	0	**ACD/LogP**	1.59
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	n1c2ccccc2oc1				
STD InChIKey	BCMCBBGGLRIHSE-UHFFFAOYAP				

Melting Points

mp °C	source
30.00	Alfa Aesar
31.00	PHYSPROP

benzoyl thiol C11H8OS[3, 61, 64]



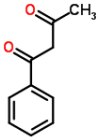
Compound Data

Melting point	**56.50 °C**	**329.65 K**			
CSID	60596	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	188.2456	**H bond donors**	0	**ACD/LogP**	2.86
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	O=C(c1ccccc1)c2sccc2				
STD InChIKey	DWYFUJJWTRPARQ-UHFFFAOYAX				

Melting Points

mp °C	source
56.00	Alfa Aesar
57.00	Oxford University MSDS
56.50	PHYSPROP

benzoylacetone C10H10O2[2, 64]



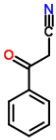
Compound Data

Melting point	**57.50 °C**	**330.65 K**			
CSID	6898	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	162.1852	**H bond donors**	0	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	O=C(c1ccccc1)CC(=O)C				
STD InChIKey	CVBUKMMMRLOKQR-UHFFFAOYAW				

Melting Points

mp °C	source
59.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
56.00	PHYSPROP

benzoylacetonitrile C9H7NO[3, 48, 64]



Compound Data

Melting point	**81.50 °C**	**354.65 K**			
CSID	58331	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	145.158	**H bond donors**	0	**ACD/LogP**	0.97
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	O=C(c1ccccc1)CC#N				
STD InChIKey	ZJRCIQAMTAINCB-UHFFFAOYAL				

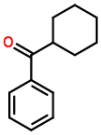
Melting Points

mp °C	source

81.00	Alfa Aesar
83.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
80.50	PHYSPROP

benzoylcyclohexane C13H16O[2, 3, 64]

Compound Data



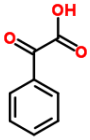
Melting point	**55.33 °C**	**328.48 K**			
CSID	12307	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	188.2655	**H bond donors**	0	**ACD/LogP**	3.73
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	O=C(c1ccccc1)C2CCCCC2				
STD InChIKey	BMFYCFSWWDXEPB-UHFFFAOYAK				

Melting Points

mp °C	source
55.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
55.00	Alfa Aesar
56.00	PHYSPROP

benzoylformic acid C8H6O3[3, 64]

Compound Data



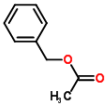
Melting point	**65.50 °C**	**338.65 K**			
CSID	11421	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1314	**H bond donors**	1	**ACD/LogP**	0.69
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.30 g/cm^3
SMILES	O=C(C(=O)O)c1ccccc1				
STD InChIKey	FAQJJMHZNSSFSM-UHFFFAOYAS				

Melting Points

mp °C	source
65.00	Alfa Aesar
66.00	PHYSPROP

benzyl acetate C9H10O2[2, 3, 64]

Compound Data



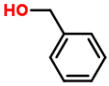
Melting point	**-51.10 °C**	**222.05 K**			
CSID	13850405	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	0	**ACD/LogP**	1.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3
SMILES	CC(=O)OCc1ccccc1				
STD InChIKey	QUKGYYKBILRGFE-UHFFFAOYAD				

Melting Points

mp °C	source
-51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-51.00	Alfa Aesar
-51.30	PHYSPROP

benzyl alcohol C7H8O[3, 31, 61, 64]

Compound Data



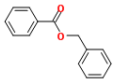
Melting point	**-15.05 °C**	**258.10 K**			
CSID	13860335	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	108.1378	**H bond donors**	1	**ACD/LogP**	1.05
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	c1ccc(cc1)CO				
STD InChIKey	WVDDGKGOMKODPV-UHFFFAOYAH				

Melting Points

mp °C	source
-15.00	Alfa Aesar
-15.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-15.00	Oxford University MSDS
-15.20	PHYSPROP

benzyl benzoate C14H12O2[2, 3, 32, 61, 64]

Compound Data



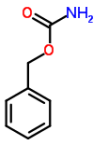
Melting point	**19.60 °C**	**292.75 K**			
CSID	13856959	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	0	**ACD/LogP**	3.97
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	O=C(OCc1ccccc1)c2ccccc2				
STD InChIKey	SESFRYSPDFLNCH-UHFFFAOYAD				

Melting Points

mp °C	source
19.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
19.00	Alfa Aesar
21.00	DrugBank
18.00	Oxford University MSDS
21.00	PHYSPROP

benzyl carbamate C8H9NO2[3, 64]

Compound Data



Melting point	**87.50 °C**	**360.65 K**			
CSID	11638	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OCc1ccccc1)N				
STD InChIKey	PUJDIJCNWFYVJX-UHFFFAOYAU				

Melting Points

mp °C	source
87.00	Alfa Aesar
88.00	PHYSPROP

benzyl chloride C7H7Cl[2, 3, 64]

Compound Data

Melting point	**-43.67 °C**	**229.48 K**			
CSID	13840690	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	126.5835	**H bond donors**	0	**ACD/LogP**	2.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	c1ccc(cc1)CCl				
STD InChIKey	KCXMKQUNVWSEMD-UHFFFAOYAV				

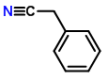
Melting Points

mp °C	source
-43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-43.00	Alfa Aesar
-45.00	PHYSPROP

benzyl cyanide C8H7N[2, 3, 64]

Compound Data

Melting point	**-23.93 °C**	**249.22 K**			
CSID	13839308	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	117.1479	**H bond donors**	0	**ACD/LogP**	1.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	3



1.01 g/cm

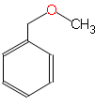
SMILES	c1ccc(cc1)CC#N
STD InChIKey	SUSQOBVLVYHIEX-UHFFFAOYAJ

Melting Points

mp °C	source
-24.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-24.00	Alfa Aesar
-23.80	PHYSPROP

benzyl methyl ether C8H10O[3, 7, 64]

Compound Data



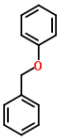
Melting point	**-52.53 °C**	**220.62 K**			
CSID	21170543	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	0	**ACD/LogP**	1.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.95 g/cm^3
SMILES	COCc1ccccc1				
STD InChIKey	GQKZBCPTCWJTAS-UHFFFAOYAD				

Melting Points

mp °C	source
-53.00	Alfa Aesar
-52.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
-52.60	PHYSPROP

benzyl phenyl ether C13H12O[3, 64]

Compound Data



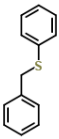
Melting point	**39.50 °C**	**312.65 K**			
CSID	63533	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.2338	**H bond donors**	0	**ACD/LogP**	3.79
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.06 g/cm^3
SMILES	O(c1ccccc1)Cc2ccccc2				
STD InChIKey	BOTNYLSAWDQNEX-UHFFFAOYAS				

Melting Points

mp °C	source
39.00	Alfa Aesar
40.00	PHYSPROP

benzyl phenyl sulfide C13H12S[3, 64]

Compound Data



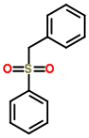
Melting point	**42.25 °C**	**315.40 K**			
CSID	12697	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	200.2994	**H bond donors**	0	**ACD/LogP**	3.80
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	S(c1ccccc1)Cc2ccccc2				
STD InChIKey	LKMCJXXOBRCATQ-UHFFFAOYAC				

Melting Points

mp °C	source
41.00	Alfa Aesar
43.50	PHYSPROP

benzyl phenyl sulfone C13H12O2S[3, 64]

Compound Data



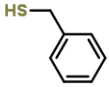
Melting point	**147.50 °C**	**420.65 K**			
CSID	69027	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	232.2982	**H bond donors**	0	**ACD/LogP**	2.35
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	O=S(=O)(c1ccccc1)Cc2ccccc2				
STD InChIKey	FABCMLOTUSCWOR-UHFFFAOYAK				

Melting Points

mp °C	source
149.00	Alfa Aesar
146.00	PHYSPROP

benzyl sulfide C7H8S[3, 17, 55, 64]

Compound Data



Melting point	**-29.55 °C**	**243.60 K**			
CSID	13851383	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	124.2034	**H bond donors**	0	**ACD/LogP**	2.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	SCc1ccccc1				
STD InChIKey	UENWRTRMUIOCKN-UHFFFAOYAC				

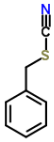
Melting Points

mp °C	source
-30.00	Alfa Aesar
-29.00	ChemBlink
-29.20	Merck Chemicals
-30.00	PHYSPROP
	Values not used in calculating the average melting point
49.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...[1]

1. clearly out of range JCB

benzyl thiocyanate C8H7NS[3, 64]

Compound Data



Melting point	**42.50 °C**	**315.65 K**			
CSID	17163	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	149.2129	**H bond donors**	0	**ACD/LogP**	1.99
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	N#CSCc1ccccc1				
STD InChIKey	ABNDFSOIUFLJAH-UHFFFAOYAN				

Melting Points

mp °C	source
42.00	Alfa Aesar
43.00	PHYSPROP

benzylbromide C7H7Br[2, 3, 61, 64]

Compound Data

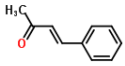
Melting point	**-3.00 °C**	**270.15 K**			
CSID	13851576	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	171.0345	**H bond donors**	0	**ACD/LogP**	2.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.44 g/cm^3
SMILES	c1ccc(cc1)CBr				
STD InChIKey	AGEZXYOZHKGVCM-UHFFFAOYAM				

Melting Points

mp °C	source
-2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-4.00	Alfa Aesar
-3.00	Oxford University MSDS

-3.00	PHYSPROP

benzylideneacetone C10H10O[2, 3, 64, 64]



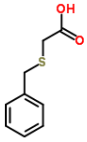
Compound Data

Melting point	**41.12 °C**	**314.27 K**			
CSID	21106584	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	146.1858	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.01 g/cm^3
SMILES	CC(=O)/C=C/c1ccccc1				
STD InChIKey	BWHOZHOGCMHOBV-BQYQJAHWBQ				

Melting Points

mp °C	source
41.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
40.00	Alfa Aesar
42.00	PHYSPROP
41.50	PHYSPROP

benzylthioacetic acid C9H10O2S[3, 64]



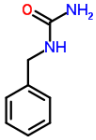
Compound Data

Melting point	**61.50 °C**	**334.65 K**			
CSID	60259	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	182.2395	**H bond donors**	1	**ACD/LogP**	2.10
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.24 g/cm^3
SMILES	O=C(O)CSCc1ccccc1				
STD InChIKey	AWLVTQRRKPBQEQ-UHFFFAOYAW				

Melting Points

mp °C	source
62.00	Alfa Aesar
61.00	PHYSPROP

benzylurea C8H10N2O[3, 64]



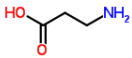
Compound Data

Melting point	**148.50 °C**	**421.65 K**			
CSID	10396	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1778	**H bond donors**	3	**ACD/LogP**	0.73
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(NCc1ccccc1)N				
STD InChIKey	RJNJWHFSKNJCTB-UHFFFAOYAZ				

Melting Points

mp °C	source
149.00	Alfa Aesar
148.00	PHYSPROP

beta-alanine C3H7NO2[35, 61]



Compound Data

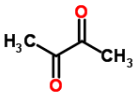
Melting point	**198.00 °C**	**471.15 K**			
CSID	234	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	89.0932	**H bond donors**	3	**ACD/LogP**	-0.86
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)CCN				
STD InChIKey	UCMIRNVEIXFBKS-UHFFFAOYAL				

Melting Points

mp °C	source
200.00	EPISuite-ChemSpider

196.00	Oxford University MSDS

biacetyl C4H6O2[3, 61, 64]



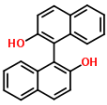
Compound Data

Melting point	**-2.40 °C**	**270.75 K**			
CSID	630	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	86.0892	**H bond donors**	0	**ACD/LogP**	-1.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	O=C(C(=O)C)C				
STD InChIKey	QSJXEFYPDANLFS-UHFFFAOYAX				

Melting Points

mp °C	source
-3.00	Alfa Aesar
-3.00	Oxford University MSDS
-1.20	PHYSPROP

binol C20H14O2[3, 48, 64]



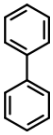
Compound Data

Melting point	**216.17 °C**	**489.32 K**			
CSID	11269	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	286.324	**H bond donors**	2	**ACD/LogP**	4.86
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.30 g/cm^3
SMILES	c1ccc2c(c1)ccc(c2c3c4ccccc4ccc3O)O				
STD InChIKey	PPTXVXKCQZKFBN-UHFFFAOYAX				

Melting Points

mp °C	source
217.00	Alfa Aesar
216.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
215.50	PHYSPROP

biphenyl C12H10[3, 4, 35, 44, 59, 64, 64, 70]



Compound Data

Melting point	**69.64 °C**	**342.79 K**			
CSID	6828	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	154.2078	**H bond donors**	0	**ACD/LogP**	4.09
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	c1ccc(cc1)c2ccccc2				
STD InChIKey	ZUOUZKKEUPVFJK-UHFFFAOYAV				

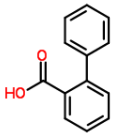
Melting Points

mp °C	source
71.00	Alfa Aesar
69.00	American Petroleum Institute. Research Project 44; Selected ...
70.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
69.85	NIST Web Book
69.00	PHYSPROP
69.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
	Values not used in calculating the average melting point
12.00	EPISuite-ChemSpider[1]
12.00	PHYSPROP[2]

1. value clearly out of range JCB
2. clearly out of range JCB

biphenyl-2-carboxylic acid C13H10O2[3, 7, 64]

Compound Data



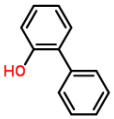
Melting point	**113.77 °C**	**386.92 K**			
CSID	63538	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2173	**H bond donors**	1	**ACD/LogP**	3.00
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	O=C(O)c2ccccc2c1ccccc1				
STD InChIKey	ILYSAKHOYBPSPC-UHFFFAOYAU				

Melting Points

mp °C	source
112.00	Alfa Aesar
115.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
114.30	PHYSPROP

biphenyl-2-ol C12H10O[2, 3, 61, 64]

Compound Data



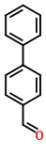
Melting point	**58.00 °C**	**331.15 K**			
CSID	13839012	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2072	**H bond donors**	1	**ACD/LogP**	2.94
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	Oc2ccccc2c1ccccc1				
STD InChIKey	LLEMOWNGBBNAJR-UHFFFAOYAF				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
56.00	Alfa Aesar
57.00	Oxford University MSDS
59.00	PHYSPROP

biphenyl-4-carboxaldehyde C13H10O[3, 7]

Compound Data



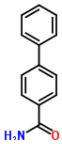
Melting point	**59.50 °C**	**332.65 K**			
CSID	69150	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.2179	**H bond donors**	0	**ACD/LogP**	3.83
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	O=Cc2ccc(c1ccccc1)cc2				
STD InChIKey	ISDBWOPVZKNQDW-UHFFFAOYAQ				

Melting Points

mp °C	source
59.00	Alfa Aesar
60.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

biphenyl-4-carboxamide C13H11NO[3, 7]

Compound Data

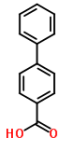


Melting point	**225.50 °C**	**498.65 K**			
CSID	523754	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	197.2325	**H bond donors**	2	**ACD/LogP**	2.93
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(c2ccc(c1ccccc1)cc2)N				
STD InChIKey	LUQVCHRDAGWYMG-UHFFFAOYAA				

Melting Points

mp °C	source
228.00	Alfa Aesar
223.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....

biphenyl-4-carboxylic acid C13H10O2[3, 7, 64]



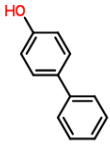
Compound Data

Melting point	**226.67 °C**	**499.82 K**			
CSID	60090	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2173	**H bond donors**	1	**ACD/LogP**	3.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	O=C(O)c2ccc(c1ccccc1)cc2				
STD InChIKey	NNJMFJSKMRYHSR-UHFFFAOYAD				

Melting Points

mp °C	source
225.00	Alfa Aesar
227.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
228.00	PHYSPROP

biphenyl-4-ol C12H10O[2, 3, 61, 64, 72]



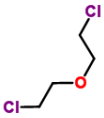
Compound Data

Melting point	**166.20 °C**	**439.35 K**			
CSID	13846658	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2072	**H bond donors**	1	**ACD/LogP**	3.45
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	c1ccc(cc1)c2ccc(cc2)O				
STD InChIKey	YXVFYQXJAXKLAK-UHFFFAOYAY				

Melting Points

mp °C	source
167.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
166.00	Alfa Aesar
167.00	Oxford University MSDS
166.00	PHYSPROP
165.00	Sigma-Aldrich

bis(2-chloroethyl) ether C4H8Cl2O[3, 61, 64]



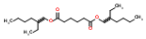
Compound Data

Melting point	**-49.63 °C**	**223.52 K**			
CSID	21106016	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.0117	**H bond donors**	0	**ACD/LogP**	1.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.16 g/cm^3
SMILES	ClCCOCCCl				
STD InChIKey	ZNSMNVMLTJELDZ-UHFFFAOYAN				

Melting Points

mp °C	source
-50.00	Alfa Aesar
-47.00	Oxford University MSDS
-51.90	PHYSPROP

bis(2-ethylhexyl) adipate C22H42O4[3, 64]



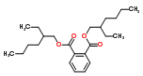
Compound Data

Melting point	**-67.40 °C**	**205.75 K**			
CSID	7358	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	370.5665	**H bond donors**	0	**ACD/LogP**	8.10
Phase 25 °C	liquid/gas	**Rotatable bonds**	19	**Predicted density**	0.93 g/cm^3
SMILES	O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CCCC)CC				
STD InChIKey	SAOKZLXYCUGLFA-UHFFFAOYAQ				

Melting Points

mp °C	source
-67.00	Alfa Aesar
-67.80	PHYSPROP

bis(2-ethylhexyl) phthalate C24H38O4[2, 3, 64]



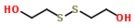
Compound Data

Melting point	**-53.33 °C 219.82 K**				
CSID	21106505	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	390.5561	**H bond donors**	0	**ACD/LogP**	8.52
Phase 25 °C	liquid/gas	**Rotatable bonds**	16	**Predicted density**	0.98 g/cm^3
SMILES	CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC				
STD InChIKey	BJQHLKABXJIVAM-UHFFFAOYAB				

Melting Points

mp °C	source
-50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-55.00	Alfa Aesar
-55.00	PHYSPROP

bis(2-hydroxyethyl) disulfide C4H10O2S2[3, 32, 64]



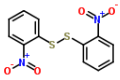
Compound Data

Melting point	**25.67 °C 298.82 K**				
CSID	15117	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	154.251	**H bond donors**	2	**ACD/LogP**	0.52
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.31 g/cm^3
SMILES	OCCSSCCO				
STD InChIKey	KYNFOMQIXZUKRK-UHFFFAOYAC				

Melting Points

mp °C	source
25.00	Alfa Aesar
26.00	DrugBank
26.00	PHYSPROP

bis(2-nitrophenyl) disulfide C12H8N2O4S2[3, 64]



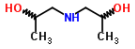
Compound Data

Melting point	**195.25 °C 468.40 K**				
CSID	64024	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	308.3329	**H bond donors**	0	**ACD/LogP**	3.37
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.52 g/cm^3
SMILES	[O-][N+](=O)c2c(SSc1ccccc1[N+]([O-])=O)cccc2				
STD InChIKey	NXCKJENHTITELM-UHFFFAOYAN				

Melting Points

mp °C	source
194.00	Alfa Aesar
196.50	PHYSPROP

bis(2-propanol)amine C6H15NO2[3, 64]



Compound Data

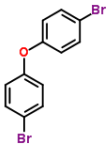
Melting point	**43.25 °C 316.40 K**				
CSID	7795	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	133.1888	**H bond donors**	3	**ACD/LogP**	-0.81
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.01 g/cm^3
SMILES	OC(C)CNCC(O)C				
STD InChIKey	LVTYICIALWPMFW-UHFFFAOYAD				

Melting Points

mp °C	source
42.00	Alfa Aesar
44.50	PHYSPROP

bis(4-bromophenyl) ether C12H8Br2O[3, 7, 64]

Compound Data



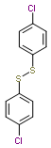
Melting point	**59.50 °C**	**332.65 K**			
CSID	15471	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	327.9993	**H bond donors**	0	**ACD/LogP**	6.01
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.70 g/cm^3
SMILES	Brc2ccc(Oc1ccc(Br)cc1)cc2				
STD InChIKey	YAWIAFUBXXPJMQ-UHFFFAOYAV				

Melting Points

mp °C	source
58.00	Alfa Aesar
60.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
60.50	PHYSPROP

bis(4-chlorophenyl) disulfide C12H8Cl2S2[3, 64]

Compound Data



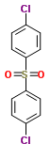
Melting point	**70.50 °C**	**343.65 K**			
CSID	13721	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	287.2279	**H bond donors**	0	**ACD/LogP**	6.02
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.43 g/cm^3
SMILES	c1cc(ccc1SSc2ccc(cc2)Cl)Cl				
STD InChIKey	ZIXXRXGPBFMPFD-UHFFFAOYAI				

Melting Points

mp °C	source
73.00	Alfa Aesar
68.00	PHYSPROP

bis(4-chlorophenyl) sulfone C12H8Cl2O2S[3, 64]

Compound Data



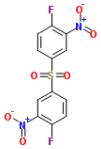
Melting point	**148.45 °C**	**421.60 K**			
CSID	6373	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	287.1617	**H bond donors**	0	**ACD/LogP**	4.20
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.42 g/cm^3
SMILES	O=S(=O)(c1ccc(Cl)cc1)c2ccc(Cl)cc2				
STD InChIKey	GPAPPPVRLPGFEQ-UHFFFAOYAQ				

Melting Points

mp °C	source
149.00	Alfa Aesar
147.90	PHYSPROP

bis(4-fluoro-3-nitrophenyl) sulfone C12H6F2N2O6S[3, 64]

Compound Data

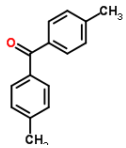


Melting point	**193.75 °C**	**466.90 K**			
CSID	9028	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	344.2476	**H bond donors**	0	**ACD/LogP**	3.23
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.64 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1F)S(=O)(=O)c2cc([N+]([O-])=O)c(F)cc2				
STD InChIKey	KHAWDEWNXJIVCJ-UHFFFAOYAC				

Melting Points

mp °C	source
194.00	Alfa Aesar
193.50	PHYSPROP

bis(4-tolyl)ketone C15H14O[3, 64]



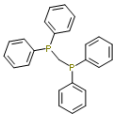
Compound Data

Melting point	**95.25 °C**	**368.40 K**			
CSID	62363	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	210.2711	**H bond donors**	0	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	O=C(c1ccc(cc1)C)c2ccc(cc2)C				
STD InChIKey	ZWPWLKXZYNXATK-UHFFFAOYAV				

Melting Points

mp °C	source
94.00	Alfa Aesar
96.50	PHYSPROP

bis(diphenylphosphino)methane C25H22P2[3, 48]



Compound Data

Melting point	**120.00 °C**	**393.15 K**			
CSID	67509	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	384.3897	**H bond donors**	0	**ACD/LogP**	8.57
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	0.00 g/cm^3
SMILES	P(c1ccccc1)(c2ccccc2)CP(c3ccccc3)c4ccccc4				
STD InChIKey	XGCDBGRZEKYHNV-UHFFFAOYAH				

Melting Points

mp °C	source
119.00	Alfa Aesar
121.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

bis(pentabromophenyl) ether C12Br10O[3, 64]

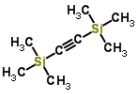
Compound Data

Melting point	**305.50 °C**	**578.65 K**			
CSID	13764	**H bond acceptors**	1	**Rule of 5 violations**	2
Molecular weight	959.1678	**H bond donors**	0	**ACD/LogP**	11.24
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.98 g/cm^3
SMILES	Brc2c(Oc1c(Br)c(Br)c(Br)c(Br)c1Br)c(Br)c(Br)c(Br)c2Br				
STD InChIKey	WHHGLZMJPXIBIX-UHFFFAOYAY				

Melting Points

mp °C	source
306.00	Alfa Aesar
305.00	PHYSPROP

bis(trimethylsilyl)acetylene C8H18Si2[3, 64]



Compound Data

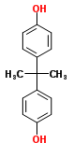
Melting point	**24.00 °C**	**297.15 K**			
CSID	76286	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	170.3995	**H bond donors**	0	**ACD/LogP**	4.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.79 g/cm^3
SMILES	C(#C[Si](C)(C)C)[Si](C)(C)C				
STD InChIKey	ZDWYFWIBTZJGOR-UHFFFAOYAF				

Melting Points

mp °C	source
22.00	Alfa Aesar
26.00	PHYSPROP

bisphenol A C15H16O2[3, 64]

Compound Data



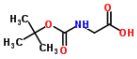
Melting point	**154.50 °C**	**427.65 K**			
CSID	6371	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	228.2863	**H bond donors**	2	**ACD/LogP**	3.64
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.14 g/cm^3
SMILES	CC(C)(c1ccc(cc1)O)c2ccc(cc2)O				
STD InChIKey	IISBACLAFKSPIT-UHFFFAOYAI				

Melting Points

mp °C	source
156.00	Alfa Aesar
153.00	PHYSPROP

boc-glycine C7H13NO4[3, 3, 72]

Compound Data



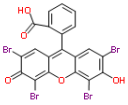
Melting point	**88.33 °C**	**361.48 K**			
CSID	70660	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	175.1824	**H bond donors**	2	**ACD/LogP**	0.75
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.16 g/cm^3
SMILES	O=C(OC(C)(C)C)NCC(=O)O				
STD InChIKey	VRPJIFMKZZEXLR-UHFFFAOYAN				

Melting Points

mp °C	source
89.00	Alfa Aesar
88.50	Alfa Aesar
87.50	Sigma-Aldrich

bromeosin C20H8Br4O5[61, 64]

Compound Data



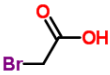
Melting point	**297.75 °C**	**570.90 K**			
CSID	10581	**H bond acceptors**	5	**Rule of 5 violations**	2
Molecular weight	647.8905	**H bond donors**	2	**ACD/LogP**	6.36
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	2.41 g/cm^3
SMILES	O=C(O)c4ccccc4C=1c3cc(Br)c(O)c(Br)c3OC=2C=1\C=C(\Br)C(=O)C=2Br				
STD InChIKey	AZXGXVQWEUFULR-UHFFFAOYAC				

Melting Points

mp °C	source
300.00	Oxford University MSDS
295.50	PHYSPROP

bromoacetic acid C2H3BrO2[3, 32, 64]

Compound Data



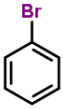
Melting point	**49.00 °C**	**322.15 K**			
CSID	10301338	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.948	**H bond donors**	1	**ACD/LogP**	0.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.00 g/cm^3
SMILES	BrCC(O)=O				
STD InChIKey	KDPAWGWELVVRCH-UHFFFAOYAM				

Melting Points

mp °C	source
47.00	Alfa Aesar
50.00	DrugBank
50.00	PHYSPROP

bromobenzene C6H5Br[3, 31, 61, 64]

Compound Data



Melting point	**-30.90 °C**	**242.25 K**			
CSID	7673	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	157.0079	**H bond donors**	0	**ACD/LogP**	2.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	c1ccc(cc1)Br				
STD InChIKey	QARVLSVVCXYDNA-UHFFFAOYAB				

Melting Points

mp °C	source
-31.00	Alfa Aesar
-31.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-31.00	Oxford University MSDS
-30.60	PHYSPROP

bromochloromethane CH2BrCl[2, 61, 64]

Compound Data

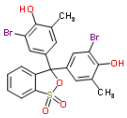
Melting point	**-87.97 °C**	**185.18 K**			
CSID	6093	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	129.3836	**H bond donors**	0	**ACD/LogP**	1.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.86 g/cm^3
SMILES	BrCCl				
STD InChIKey	JPOXNPPZZKNXOV-UHFFFAOYAI				

Melting Points

mp °C	source
-88.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-88.00	Oxford University MSDS
-87.90	PHYSPROP

bromocresol purple C21H16Br2O5S[61, 64]

Compound Data



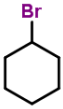
Melting point	**241.25 °C**	**514.40 K**			
CSID	7974	**H bond acceptors**	5	**Rule of 5 violations**	2
Molecular weight	540.2217	**H bond donors**	2	**ACD/LogP**	5.92
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.77 g/cm^3
SMILES	Brc1c(O)c(cc(c1)C3(OS(=O)(=O)c2ccccc23)c4cc(c(O)c(Br)c4)C)C				
STD InChIKey	ABIUHPWEYMSGSR-UHFFFAOYAH				

Melting Points

mp °C	source
241.00	Oxford University MSDS
241.50	PHYSPROP

bromocyclohexane C6H11Br[3, 64]

Compound Data



Melting point	**-56.75 °C**	**216.40 K**			
CSID	7672	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	163.0555	**H bond donors**	0	**ACD/LogP**	3.21
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.35 g/cm^3
SMILES	BrC1CCCCC1				
STD InChIKey	AQNQQHJNRPDOQV-UHFFFAOYAD				

Melting Points

mp °C	source
-57.00	Alfa Aesar
-56.50	PHYSPROP

bromodichloromethane CHBrCl2[2, 3, 64]

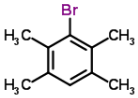
Compound Data

Melting point	**-56.33 °C**	**216.82 K**			
CSID	6119	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	163.8286	**H bond donors**	0	**ACD/LogP**	2.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.01 g/cm^3
SMILES	BrC(Cl)Cl				
STD InChIKey	FMWLUWPQPKEARP-UHFFFAOYAR				

Melting Points

mp °C	source
-55.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-57.00	Alfa Aesar
-57.00	PHYSPROP

bromodurene C10H13Br[3, 48]



Compound Data

Melting point	**58.00 °C**	**331.15 K**			
CSID	66847	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	213.1142	**H bond donors**	0	**ACD/LogP**	4.83
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	Brc1c(c(cc(c1C)C)C)C				
STD InChIKey	WJKBPTLQJXKEHC-UHFFFAOYAB				

Melting Points

mp °C	source
60.00	Alfa Aesar
56.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

bromoethane C2H5Br[2, 3, 31, 61, 64]

Compound Data

Melting point	**-118.92 °C**	**154.23 K**			
CSID	6092	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	108.9651	**H bond donors**	0	**ACD/LogP**	1.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.46 g/cm^3
SMILES	BrCC				
STD InChIKey	RDHPKYGYEGBMSE-UHFFFAOYAC				

Melting Points

mp °C	source
-119.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-119.00	Alfa Aesar
-119.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-119.00	Oxford University MSDS
-118.60	PHYSPROP

bromoethene C2H3Br[61, 64]

Compound Data

Melting point	**-138.40 °C**	**134.75 K**			
CSID	11151	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.9492	**H bond donors**	0	**ACD/LogP**	1.57
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.53 g/cm^3
SMILES	C=CBr				
STD InChIKey	INLLPKCGLOXCIV-UHFFFAOYAI				

Melting Points

mp °C	source
-139.00	Oxford University MSDS
-137.80	PHYSPROP

bromoform $CHBr_3$[2, 3, 61, 64]

Compound Data

Melting point	**8.50 °C**	**281.65 K**			
CSID	13838404	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	252.7306	**H bond donors**	0	**ACD/LogP**	2.29
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.97 g/cm^3
SMILES	BrC(Br)Br				
STD InChIKey	DIKBFYAXUHHXCS-UHFFFAOYAM				

Melting Points

mp °C	source
8.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
9.00	Alfa Aesar
9.00	Oxford University MSDS
8.00	PHYSPROP

bromopentamethylbenzene $C_{11}H_{15}Br$[3, 48]

Compound Data

Melting point	**163.50 °C**	**436.65 K**			
CSID	71166	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	227.1408	**H bond donors**	0	**ACD/LogP**	5.29
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.21 g/cm^3
SMILES	Brc1c(c(c(c(c1C)C)C)C)C				
STD InChIKey	XPDQRULPGCFCLX-UHFFFAOYAA				

Melting Points

mp °C	source
162.00	Alfa Aesar
165.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

bromotrichloromethane $CBrCl_3$[3, 64]

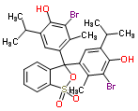
Compound Data

Melting point	**-5.85 °C**	**267.30 K**			
CSID	6143	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	198.2737	**H bond donors**	0	**ACD/LogP**	3.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.15 g/cm^3
SMILES	BrC(Cl)(Cl)Cl				
STD InChIKey	XNNQFQFUQLJSQT-UHFFFAOYAX				

Melting Points

mp °C	source
-6.00	Alfa Aesar
-5.70	PHYSPROP

bromthymol blue $C_{27}H_{28}Br_2O_5S$[3, 61, 64]



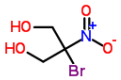
Compound Data

Melting point	**200.67 °C**	**473.82 K**			
CSID	6208	**H bond acceptors**	5	**Rule of 5 violations**	2
Molecular weight	624.3812	**H bond donors**	2	**ACD/LogP**	8.60
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.54 g/cm^3
SMILES	Brc1c(O)c(cc(c1C)C3(OS(=O)(=O)c2ccccc23)c4cc(c(O)c(Br)c4C)C(C)C)C(C)C				
STD InChIKey	NUHCTOLBWMJMLX-UHFFFAOYAD				

Melting Points

mp °C	source
201.00	Alfa Aesar
200.00	Oxford University MSDS
201.00	PHYSPROP

bronopol C3H6BrNO4[3, 64]



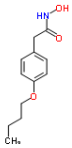
Compound Data

Melting point	**129.25 °C**	**402.40 K**			
CSID	2356	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	199.988	**H bond donors**	2	**ACD/LogP**	1.72
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	2.02 g/cm^3
SMILES	[O-][N+](=O)C(Br)(CO)CO				
STD InChIKey	LVDKZNITIUWNER-UHFFFAOYAZ				

Melting Points

mp °C	source
127.00	Alfa Aesar
131.50	PHYSPROP

bufexamac C12H17NO3[9, 48, 64]



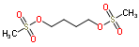
Compound Data

Melting point	**153.33 °C**	**426.48 K**			
CSID	2372	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	223.2683	**H bond donors**	2	**ACD/LogP**	1.70
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.12 g/cm^3
SMILES	O=C(NO)Cc1ccc(OCCCC)cc1				
STD InChIKey	MXJWRABVEGLYDG-UHFFFAOYAY				

Melting Points

mp °C	source
153.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
153.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
154.00	PHYSPROP

busulfan C6H14O6S2[44, 64, 72]



Compound Data

Melting point	**115.83 °C**	**388.98 K**			
CSID	2384	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	246.3018	**H bond donors**	0	**ACD/LogP**	-0.52
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.35 g/cm^3
SMILES	O=S(=O)(OCCCCOS(=O)(=O)C)C				
STD InChIKey	COVZYZSDYWQREU-UHFFFAOYAO				

Melting Points

mp °C	source
116.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
116.00	PHYSPROP
115.50	Sigma-Aldrich
	Values not used in calculating the average melting point
287.00	DrugBank[1]

1. clearly out of range JCB

butadiene C4H6[61, 64]

Compound Data

Melting point	**-110.95 °C**	**162.20 K**			
CSID	7557	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	54.0904	**H bond donors**	0	**ACD/LogP**	1.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.64 g/cm^3
SMILES	C=CC=C				
STD InChIKey	KAKZBPTYRLMSJV-UHFFFAOYAZ				

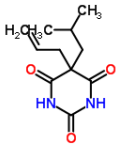
Melting Points

mp °C	source

-113.00	Oxford University MSDS
-108.90	PHYSPROP

butalbital C11H16N2O3[9, 32, 44, 48, 64]

Compound Data



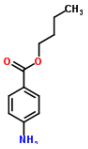
Melting point	**138.60 °C**	**411.75 K**			
CSID	2387	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	224.2563	**H bond donors**	2	**ACD/LogP**	1.65
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.08 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(CC(C)C)C\C=C				
STD InChIKey	UZVHFVZFNXBMQJ-UHFFFAOYAQ				

Melting Points

mp °C	source
138.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
138.50	DrugBank
140.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
138.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
138.50	PHYSPROP

butamben C11H15NO2[44, 64, 70, 72, 72]

Compound Data



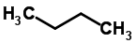
Melting point	**57.80 °C**	**330.95 K**			
CSID	2388	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	193.2423	**H bond donors**	2	**ACD/LogP**	3.01
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.08 g/cm^3
SMILES	O=C(OCCCC)c1ccc(N)cc1				
STD InChIKey	IUWVALYLNVXWKX-UHFFFAOYAU				

Melting Points

mp °C	source
58.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
58.00	PHYSPROP
58.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
57.50	Sigma-Aldrich
57.50	Sigma-Aldrich

butane C4H10[4, 15, 59, 64]

Compound Data



Melting point	**-137.92 °C**	**135.23 K**			
CSID	7555	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	58.1222	**H bond donors**	0	**ACD/LogP**	2.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.61 g/cm^3
SMILES	CCCC				
STD InChIKey	IJDNQMDRQITEOD-UHFFFAOYAE				

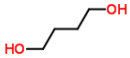
Melting Points

mp °C	source
-138.00	American Petroleum Institute. Research Project 44; Selected ...
-138.34	Carruth GF; Kobayahsi R. Journal of Chemical and Engineering...
-137.15	NIST Web Book
-138.20	PHYSPROP

butane-1,4-diol C4H10O2[2, 3, 32, 61, 64]

Compound Data

Melting point	**18.90 °C**	**292.05 K**			
CSID	13835209	**H bond acceptors**	2	**Rule of 5 violations**	0



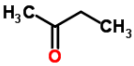
Molecular weight	90.121	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.01 g/cm^3
SMILES	C(CCO)CO				
STD InChIKey	WERYXYBDKMZEQL-UHFFFAOYAD				

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
20.00	Alfa Aesar
20.10	DrugBank
18.00	Oxford University MSDS
20.40	PHYSPROP

butanone C4H8O[3, 4, 61, 64]

Compound Data



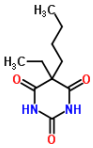
Melting point	**-86.65 °C**	**186.50 K**			
CSID	6321	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	72.1057	**H bond donors**	0	**ACD/LogP**	0.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.79 g/cm^3
SMILES	CCC(=O)C				
STD InChIKey	ZWEHNKRNPOVVGH-UHFFFAOYAW				

Melting Points

mp °C	source
-87.00	Alfa Aesar
-86.00	American Petroleum Institute. Research Project 44; Selected ...
-87.00	Oxford University MSDS
-86.60	PHYSPROP

butobarbital C10H16N2O3[32, 35, 44, 64]

Compound Data



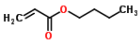
Melting point	**127.75 °C**	**400.90 K**			
CSID	6229	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	212.2456	**H bond donors**	2	**ACD/LogP**	1.71
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(CCCC)CC				
STD InChIKey	STDBAQMTJLUMFW-UHFFFAOYAW				

Melting Points

mp °C	source
128.50	DrugBank
128.50	EPISuite-ChemSpider
125.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
128.50	PHYSPROP

butyl acrylate C7H12O2[3, 64]

Compound Data



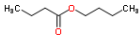
Melting point	**-64.30 °C**	**208.85 K**			
CSID	8514	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.169	**H bond donors**	0	**ACD/LogP**	2.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.90 g/cm^3
SMILES	O=C(OCCCC)\C=C				
STD InChIKey	CQEYYJKEWSMYFG-UHFFFAOYAL				

Melting Points

mp °C	source
-64.00	Alfa Aesar

-64.60	PHYSPROP

butyl butyrate C8H16O2[1, 3, 19, 28, 37, 64, 81]



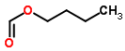
Compound Data

Melting point	**-91.79 °C**	**181.36 K**			
CSID	7694	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.2114	**H bond donors**	0	**ACD/LogP**	2.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCCCC)CCC				
STD InChIKey	XUPYJHCZDLZNFP-UHFFFAOYAI				

Melting Points

mp °C	source
-92.00	Acros
-92.00	Alfa Aesar
-92.00	Chemical Book
-91.50	CRC Handbook of Chemistry and Physics
-92.00	Fisher
-91.50	PHYSPROP
-91.50	Wikipedia

butyl formate C5H10O2[3, 64]



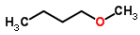
Compound Data

Melting point	**-91.75 °C**	**181.40 K**			
CSID	11125	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	0	**ACD/LogP**	1.36
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.89 g/cm^3
SMILES	O=COCCCC				
STD InChIKey	NMJJFJNHVMGPGM-UHFFFAOYAQ				

Melting Points

mp °C	source
-92.00	Alfa Aesar
-91.50	PHYSPROP

butyl methyl ether C5H12O[4, 64]



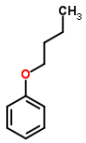
Compound Data

Melting point	**-115.25 °C**	**157.90 K**			
CSID	11833	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	0	**ACD/LogP**	1.51
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.75 g/cm^3
SMILES	O(CCCC)C				
STD InChIKey	CXBDYQVECUFKRK-UHFFFAOYAP				

Melting Points

mp °C	source
-115.00	American Petroleum Institute. Research Project 44; Selected ...
-115.50	PHYSPROP

butyl phenyl ether C10H14O[2, 3, 64]



Compound Data

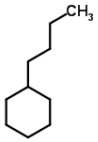
Melting point	**-19.13 °C**	**254.02 K**			
CSID	13673	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	0	**ACD/LogP**	3.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.92 g/cm^3
SMILES	O(c1ccccc1)CCCC				
STD InChIKey	YFNONBGXNFCTMM-UHFFFAOYAF				

Melting Points

mp °C	source
-19.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-19.00	Alfa Aesar
-19.40	PHYSPROP

butylcyclohexane C10H20[3, 4, 61, 64]

Compound Data



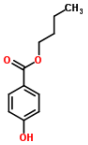
Melting point	**-75.67 °C**	**197.47 K**			
CSID	14753	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	140.2658	**H bond donors**	0	**ACD/LogP**	5.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.79 g/cm^3
SMILES	C(CCC1CCCCC1)C				
STD InChIKey	GGBJHURWWWLEQH-UHFFFAOYAB				

Melting Points

mp °C	source
-78.00	Alfa Aesar
-75.00	American Petroleum Institute. Research Project 44; Selected ...
-75.00	Oxford University MSDS
-74.70	PHYSPROP

butylparaben C11H14O3[3, 35, 44, 48, 61, 64, 70, 72, 72]

Compound Data



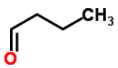
Melting point	**69.06 °C**	**342.21 K**			
CSID	6916	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	194.2271	**H bond donors**	1	**ACD/LogP**	3.46
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.11 g/cm^3
SMILES	O=C(OCCCC)c1ccc(O)cc1				
STD InChIKey	QFOHBWFCKVYLES-UHFFFAOYAN				

Melting Points

mp °C	source
69.00	Alfa Aesar
68.50	EPISuite-ChemSpider
68.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
72.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
68.50	Oxford University MSDS
68.50	PHYSPROP
69.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
68.50	Sigma-Aldrich
69.00	Sigma-Aldrich

butyraldehyde C4H8O[3, 4, 61, 64]

Compound Data

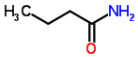


Melting point	**-97.75 °C**	**175.40 K**			
CSID	256	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	72.1057	**H bond donors**	0	**ACD/LogP**	0.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.78 g/cm^3
SMILES	O=CCCC				
STD InChIKey	ZTQSAGDEMFDKMZ-UHFFFAOYAZ				

Melting Points

mp °C	source
-99.00	Alfa Aesar
-97.00	American Petroleum Institute. Research Project 44; Selected ...
-96.00	Oxford University MSDS
-99.00	PHYSPROP

butyramide C4H9NO[2, 3, 32, 64]



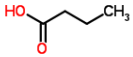
Compound Data

Melting point	**115.15 °C**	**388.30 K**			
CSID	10464	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	87.1204	**H bond donors**	2	**ACD/LogP**	-0.17
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.91 g/cm^3
SMILES	O=C(N)CCC				
STD InChIKey	DNSISZSEWVHGLH-UHFFFAOYAW				

Melting Points

mp °C	source
116.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
115.00	Alfa Aesar
114.80	DrugBank
114.80	PHYSPROP

butyric acid C4H8O2[3, 4, 35, 61, 64]



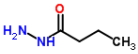
Compound Data

Melting point	**-6.32 °C**	**266.83 K**			
CSID	259	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	1	**ACD/LogP**	0.70
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	CCCC(=O)O				
STD InChIKey	FERIUCNNQQJTOY-UHFFFAOYAP				

Melting Points

mp °C	source
-8.00	Alfa Aesar
-5.00	American Petroleum Institute. Research Project 44; Selected ...
-5.70	EPISuite-ChemSpider
-5.00	Oxford University MSDS
-7.90	PHYSPROP

butyric acid hydrazide C4H10N2O[3, 64]



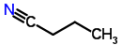
Compound Data

Melting point	**44.75 °C**	**317.90 K**			
CSID	69525	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	102.135	**H bond donors**	3	**ACD/LogP**	-0.57
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.98 g/cm^3
SMILES	O=C(NN)CCC				
STD InChIKey	FCCCRBDJBTVFSJ-UHFFFAOYAB				

Melting Points

mp °C	source
44.00	Alfa Aesar
45.50	PHYSPROP

butyronitrile C4H7N[3, 31, 64]



Compound Data

Melting point	**-111.97 °C**	**161.18 K**			
CSID	7717	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	69.1051	**H bond donors**	0	**ACD/LogP**	0.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.79 g/cm^3
SMILES	CCCC#N				
STD InChIKey	KVNRLNFWIYMESJ-UHFFFAOYAM				

Melting Points

mp °C	source

-112.00	Alfa Aesar
-112.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-111.90	PHYSPROP

caffeine C8H10N4O2[3, 32, 35, 44, 61, 64, 64, 70]

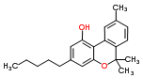
Compound Data

Melting point	**237.50 °C**	**510.65 K**			
CSID	2424	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	194.1906	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.46 g/cm^3
SMILES	Cn1cnc2c1c(=O)n(c(=O)n2C)C				
STD InChIKey	RYYVLZVUVIJVGH-UHFFFAOYAW				

Melting Points

mp °C	source
235.00	Alfa Aesar
238.00	DrugBank
238.00	EPISuite-ChemSpider
238.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
237.00	Oxford University MSDS
238.00	PHYSPROP
238.00	PHYSPROP
238.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

cannabinol C21H26O2[61, 64]



Compound Data

Melting point	**76.75 °C**	**349.90 K**			
CSID	2447	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	310.4299	**H bond donors**	1	**ACD/LogP**	7.35
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.06 g/cm^3
SMILES	Oc2cc(cc1OC(c3c(c12)cc(cc3)C)(C)C)CCCCC				
STD InChIKey	VBGLYOIFKLUMQG-UHFFFAOYAM				

Melting Points

mp °C	source
76.50	Oxford University MSDS
77.00	PHYSPROP

caprolactam C6H11NO[3, 61, 64]

Compound Data

Melting point	**69.43 °C**	**342.58 K**			
CSID	7480	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	113.1576	**H bond donors**	1	**ACD/LogP**	-0.32
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.97 g/cm^3
SMILES	O=C1NCCCCC1				
STD InChIKey	JBKVHLHDHHXQEQ-UHFFFAOYAF				

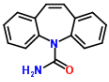
Melting Points

mp °C	source
70.00	Alfa Aesar
69.00	Oxford University MSDS
69.30	PHYSPROP

carbamazepine C15H12N2O[9, 28, 32, 35, 44, 48, 56, 64, 72]

Compound Data

Melting point	**190.59 °C**	**463.74 K**			
CSID	2457	**H bond acceptors**	3	**Rule of 5 violations**	0



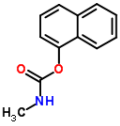
Molecular weight	236.2686	**H bond donors**	2	**ACD/LogP**	1.90
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	c1ccc2c(c1)C=Cc3ccccc3N2C(=O)N				
STD InChIKey	FFGPTBGBLSHEPO-UHFFFAOYAM				

Melting Points

mp °C	source
190.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
190.20	CRC Handbook of Chemistry and Physics
190.20	DrugBank
190.20	EPISuite-ChemSpider
191.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
190.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
191.50	Merck Index
190.20	PHYSPROP
191.50	Sigma-Aldrich

carbaryl C12H11NO2[9, 48, 61, 64]

Compound Data



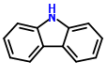
Melting point	**142.75 °C**	**415.90 K**			
CSID	5899	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	201.2212	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	O=C(Oc2cccc1ccccc12)NC				
STD InChIKey	CVXBEEMKQHEXEN-UHFFFAOYAZ				

Melting Points

mp °C	source
142.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
142.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
142.00	Oxford University MSDS
145.00	PHYSPROP

carbazole C12H9N[3, 61, 64]

Compound Data



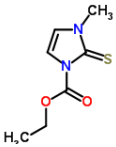
Melting point	**244.90 °C**	**518.05 K**			
CSID	6593	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	167.2066	**H bond donors**	1	**ACD/LogP**	3.76
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3
SMILES	c1ccc2c(c1)c3ccccc3[nH]2				
STD InChIKey	UJOBWOGCFQCDNV-UHFFFAOYAV				

Melting Points

mp °C	source
243.00	Alfa Aesar
245.50	Oxford University MSDS
246.20	PHYSPROP

carbimazole C7H10N2O2S[3, 32, 64]

Compound Data



Melting point	**123.67 °C**	**396.82 K**			
CSID	28829	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	186.2315	**H bond donors**	0	**ACD/LogP**	0.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	S=C1N(\C=C/N1C(=O)OCC)C				
STD InChIKey	CFOYWRHIYXMDOT-UHFFFAOYAV				

Melting Points

mp °C	source
124.00	Alfa Aesar
123.50	DrugBank
123.50	PHYSPROP

carbitol C6H14O3[3, 61, 64]

Compound Data

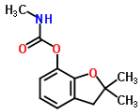
Melting point	**-77.33 °C**	**195.82 K**			
CSID	13839107	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	134.1736	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.97 g/cm^3
SMILES	OCCOCCOCC				
STD InChIKey	XXJWXESWEXIICW-UHFFFAOYAC				

Melting Points

mp °C	source
-80.00	Alfa Aesar
-76.00	Oxford University MSDS
-76.00	PHYSPROP

carbofuran C12H15NO3[44, 64]

Compound Data



Melting point	**151.25 °C**	**424.40 K**			
CSID	2468	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	221.2524	**H bond donors**	1	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(Oc2cccc1c2OC(C1)(C)C)NC				
STD InChIKey	DUEPRVBVGDRKAG-UHFFFAOYAB				

Melting Points

mp °C	source
151.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
151.00	PHYSPROP

carbon disulfide CS2[3, 61, 64]

Compound Data

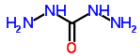
Melting point	**-111.83 °C**	**161.32 K**			
CSID	6108	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	76.1407	**H bond donors**	0	**ACD/LogP**	1.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	C(=S)=S				
STD InChIKey	QGJOPFRUJISHPQ-UHFFFAOYAS				

Melting Points

mp °C	source
-112.00	Alfa Aesar
-112.00	Oxford University MSDS
-111.50	PHYSPROP

carbonohydrazide CH6N4O[3, 61, 64]

Compound Data



Melting point	**155.83 °C**	**428.98 K**			
CSID	66578	**H bond acceptors**	5	**Rule of 5 violations**	1
Molecular weight	90.0845	**H bond donors**	6	**ACD/LogP**	-1.94
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=C(NN)NN				

STD InChIKey	XEVRDFDBXJMZFG-UHFFFAOYAS

Melting Points

mp °C	source
156.00	Alfa Aesar
157.50	Oxford University MSDS
154.00	PHYSPROP

carbonyl sulfide COS[61, 64]

Compound Data

Melting point	**-138.90 °C**	**134.25 K**			
CSID	9644	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	60.0751	**H bond donors**	0	**ACD/LogP**	0.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	O=C=S				
STD InChIKey	JJWKPURADFRFRB-UHFFFAOYAF				

Melting Points

mp °C	source
-139.00	Oxford University MSDS
-138.80	PHYSPROP

carbonyldiimidazole C7H6N4O[3, 64]

Compound Data

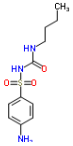
Melting point	**118.50 °C**	**391.65 K**			
CSID	61561	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	162.1487	**H bond donors**	0	**ACD/LogP**	-0.64
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.39 g/cm^3
SMILES	O=C(n1cncc1)n2ccnc2				
STD InChIKey	PFKFTWBEEFSNDU-UHFFFAOYAX				

Melting Points

mp °C	source
118.00	Alfa Aesar
119.00	PHYSPROP

carbutamide C11H17N3O3S[9, 64]

Compound Data



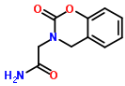
Melting point	**144.25 °C**	**417.40 K**			
CSID	9189	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	271.336	**H bond donors**	4	**ACD/LogP**	1.01
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.27 g/cm^3
SMILES	O=S(=O)(c1ccc(N)cc1)NC(=O)NCCCC				
STD InChIKey	VDTNNGKXZGSZIP-UHFFFAOYAW				

Melting Points

mp °C	source
144.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
144.50	PHYSPROP

caroxazone C10H10N2O3[9, 48, 64]

Compound Data



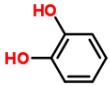
Melting point	**203.33 °C**	**476.48 K**			
CSID	27057	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	206.198	**H bond donors**	2	**ACD/LogP**	0.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=C(N)CN2C(=O)Oc1ccccc1C2				
STD InChIKey	KYCBWEZLKCTALM-UHFFFAOYAW				

Melting Points

mp °C	source
203.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
203.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
204.00	PHYSPROP

catechol C6H6O2[2, 3, 32, 61, 64]

Compound Data



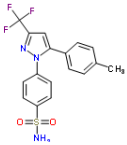
Melting point	**105.20 °C**	**378.35 K**			
CSID	13837760	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	110.1106	**H bond donors**	2	**ACD/LogP**	0.84
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	c1ccc(c(c1)O)O				
STD InChIKey	YCIMNLLNPGFGHC-UHFFFAOYAA				

Melting Points

mp °C	source
105.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
106.00	Alfa Aesar
105.00	DrugBank
105.00	Oxford University MSDS
105.00	PHYSPROP

celecoxib C17H14F3N3O2S[32, 35, 64]

Compound Data



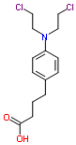
Melting point	**157.83 °C**	**430.98 K**			
CSID	2562	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	381.3722	**H bond donors**	2	**ACD/LogP**	3.90
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.43 g/cm^3
SMILES	O=S(=O)(c3ccc(n1nc(cc1c2ccc(cc2)C)C(F)(F)F)cc3)N				
STD InChIKey	RZEKVGVHFLEQIL-UHFFFAOYAD				

Melting Points

mp °C	source
157.50	DrugBank
158.00	EPISuite-ChemSpider
158.00	PHYSPROP

chlorambucil C14H19Cl2NO2[61, 64]

Compound Data



Melting point	**64.50 °C**	**337.65 K**			
CSID	2607	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	304.2122	**H bond donors**	1	**ACD/LogP**	2.61
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.25 g/cm^3
SMILES	c1cc(ccc1CCCC(=O)O)N(CCCl)CCCl				
STD InChIKey	JCKYGMPEJWAADB-UHFFFAOYAO				

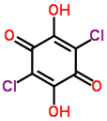
Melting Points

mp °C	source
64.00	Oxford University MSDS
65.00	PHYSPROP

chloranilic acid C6H2Cl2O4[61, 64]

Compound Data

Melting point	**283.25 °C**	**556.40 K**			
CSID	59971	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	208.9837	**H bond donors**	2	**ACD/LogP**	0.18



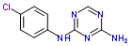
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.93 g/cm
SMILES	Cl\C1=C(/O)C(=O)C(\Cl)=C(\O)C1=O				
STD InChIKey	IPPWILKGXFOXHO-UHFFFAOYAU				

Melting Points

mp °C	source
283.00	Oxford University MSDS
283.50	PHYSPROP

chlorazanil C9H8ClN5[9, 48, 64]

Compound Data



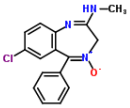
Melting point	**233.17 °C**	**506.32 K**			
CSID	9946	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	221.6463	**H bond donors**	3	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.48 g/cm^3
SMILES	Clc1ccc(cc1)Nc2ncnc(n2)N				
STD InChIKey	YRZQHIVOIFJEEE-UHFFFAOYAZ				

Melting Points

mp °C	source
233.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
233.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
233.50	PHYSPROP

chlordiazepoxide C16H14ClN3O[44, 64]

Compound Data



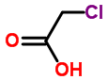
Melting point	**236.10 °C**	**509.25 K**			
CSID	10248513	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	299.7549	**H bond donors**	1	**ACD/LogP**	2.16
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	Clc1ccc2\N=C(/C[N+](/[O-])=C(\c2c1)c3ccccc3)NC				
STD InChIKey	ANTSCNMPPGJYLG-UHFFFAOYAM				

Melting Points

mp °C	source
236.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
236.20	PHYSPROP

chloroacetic acid C2H3ClO2[3, 3, 61, 64]

Compound Data

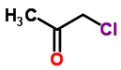


Melting point	**62.38 °C**	**335.52 K**			
CSID	10772140	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.497	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	ClCC(O)=O				
STD InChIKey	FOCAUTSVDIKZOP-UHFFFAOYAR				

Melting Points

mp °C	source
61.50	Alfa Aesar
62.00	Alfa Aesar
63.00	Oxford University MSDS
63.00	PHYSPROP

chloroacetone C3H5ClO[3, 32, 61, 64]



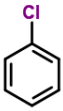
Compound Data

Melting point	**-44.62 °C**	**228.52 K**			
CSID	6323	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	92.5242	**H bond donors**	0	**ACD/LogP**	0.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	ClCC(=O)C				
STD InChIKey	BULLHNJGPPOUOX-UHFFFAOYAY				

Melting Points

mp °C	source
-45.00	Alfa Aesar
-44.50	DrugBank
-44.50	Oxford University MSDS
-44.50	PHYSPROP

chlorobenzene C6H5Cl[3, 31, 61, 64]



Compound Data

Melting point	**-45.33 °C**	**227.82 K**			
CSID	7676	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.5569	**H bond donors**	0	**ACD/LogP**	2.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c1ccc(cc1)Cl				
STD InChIKey	MVPPADPHJFYWMZ-UHFFFAOYAG				

Melting Points

mp °C	source
-45.00	Alfa Aesar
-46.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-45.00	Oxford University MSDS
-45.31	PHYSPROP

chlorocyclopropylmethane C4H7Cl[3, 64]

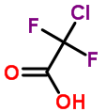
Compound Data

Melting point	**-90.95 °C**	**182.20 K**			
CSID	72268	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	90.5514	**H bond donors**	0	**ACD/LogP**	1.87
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.06 g/cm^3
SMILES	ClCC1CC1				
STD InChIKey	ZVTQWXCKQTUVPY-UHFFFAOYAG				

Melting Points

mp °C	source
-91.00	Alfa Aesar
-90.90	PHYSPROP

chlorodifluoroacetic acid C2HClF2O2[3, 64]



Compound Data

Melting point	**23.50 °C**	**296.65 K**			
CSID	10800462	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.4779	**H bond donors**	1	**ACD/LogP**	1.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.66 g/cm^3
SMILES	ClC(F)(F)C(O)=O				
STD InChIKey	OAWAZQITIZDJRB-UHFFFAOYAY				

Melting Points

mp °C	source
22.00	Alfa Aesar
25.00	PHYSPROP

chloroethane C2H5Cl[61, 64]

Compound Data

Melting point	**-138.85 °C**	**134.30 K**			
CSID	6097	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	64.5141	**H bond donors**	0	**ACD/LogP**	1.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.88 g/cm^3
SMILES	ClCC				
STD InChIKey	HRYZWHHZPQKTII-UHFFFAOYAJ				

Melting Points

mp °C	source
-139.00	Oxford University MSDS
-138.70	PHYSPROP

chloroform CHCl3[3, 5, 13, 28, 31, 58, 58, 61, 61, 64, 72]

Compound Data

Melting point	**-63.20 °C**	**209.95 K**			
CSID	5977	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	119.3776	**H bond donors**	0	**ACD/LogP**	1.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.50 g/cm^3
SMILES	ClC(Cl)Cl				
STD InChIKey	HEDRZPFGACZZDS-UHFFFAOYAG				

Melting Points

mp °C	source
-63.00	Alfa Aesar
-63.20	Archibald EH and McIntosh D. Journal of the American Chemica...
-63.50	Bridgman PW Journal of Chemical Physics 9(11) 794-797 (1941)
-63.41	CRC Handbook of Chemistry and Physics
-63.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-63.50	NIOSH
-63.00	NIOSH
-63.00	Oxford University MSDS
-63.00	Oxford University MSDS
-63.60	PHYSPROP
-63.00	Sigma-Aldrich

chloromethane CH3Cl[61, 64]

Compound Data

Melting point	**-97.35 °C**	**175.80 K**			
CSID	6087	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	50.4875	**H bond donors**	0	**ACD/LogP**	1.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.90 g/cm^3
SMILES	CCl				
STD InChIKey	NEHMKBQYUWJMIP-UHFFFAOYAW				

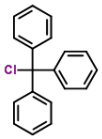
Melting Points

mp °C	source
-97.00	Oxford University MSDS
-97.70	PHYSPROP

chlorotriphenylmethane C19H15Cl[3, 64]

Compound Data

Melting point	**112.75 °C**	**385.90 K**			
CSID	6214	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	278.7754	**H bond donors**	0	**ACD/LogP**	5.57
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	ClC(c1ccccc1)(c2ccccc2)c3ccccc3				



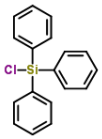
STD InChIKey	JBWKIWSBJXDJDT-UHFFFAOYAW

Melting Points

mp °C	source
112.00	Alfa Aesar
113.50	PHYSPROP

chlorotriphenylsilane C18H15ClSi[3, 64]

Compound Data



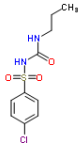
Melting point	**92.75 °C**	**365.90 K**			
CSID	6216	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	294.8502	**H bond donors**	0	**ACD/LogP**	7.43
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	Cl[Si](c1ccccc1)(c2ccccc2)c3ccccc3				
STD InChIKey	MNKYQPOFRKPUAE-UHFFFAOYAQ				

Melting Points

mp °C	source
94.00	Alfa Aesar
91.50	PHYSPROP

chlorpropamide C10H13ClN2O3S[32, 44, 61, 64]

Compound Data



Melting point	**127.95 °C**	**401.10 K**			
CSID	2626	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	276.7398	**H bond donors**	2	**ACD/LogP**	2.30
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.33 g/cm^3
SMILES	O=S(=O)(c1ccc(Cl)cc1)NC(=O)NCCC				
STD InChIKey	RKWGIWYCVPQPMF-UHFFFAOYAO				

Melting Points

mp °C	source
128.00	DrugBank
127.80	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
128.00	Oxford University MSDS
128.00	PHYSPROP

chlorpyrifos C9H11Cl3NO3PS[44, 61, 64]

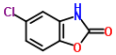
Compound Data

Melting point	**42.00 °C**	**315.15 K**			
CSID	2629	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	350.5863	**H bond donors**	0	**ACD/LogP**	4.77
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.48 g/cm^3
SMILES	Clc1c(OP(=S)(OCC)OCC)nc(Cl)c(Cl)c1				
STD InChIKey	SBPBAQFWLVIOKP-UHFFFAOYAG				

Melting Points

mp °C	source
41.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
42.50	Oxford University MSDS
42.00	PHYSPROP

chlorzoxazone C7H4ClNO2[3, 32, 64]



Compound Data

Melting point	**191.33 °C**	**464.48 K**			
CSID	2632	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	169.5652	**H bond donors**	1	**ACD/LogP**	2.19
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	Clc2cc1c(OC(=O)N1)cc2				
STD InChIKey	TZFWDZFKRBELIQ-UHFFFAOYAQ				

Melting Points

mp °C	source
191.00	Alfa Aesar
191.50	DrugBank
191.50	PHYSPROP

chromanone C9H8O2[3, 64]

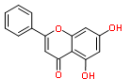
Compound Data

Melting point	**37.25 °C**	**310.40 K**			
CSID	61418	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	148.1586	**H bond donors**	0	**ACD/LogP**	1.62
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	c1ccc2c(c1)C(=O)CCO2				
STD InChIKey	MSTDXOZUKAQDRL-UHFFFAOYAG				

Melting Points

mp °C	source
38.00	Alfa Aesar
36.50	PHYSPROP

chrysin C15H10O4[3, 64]



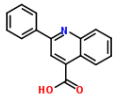
Compound Data

Melting point	**286.25 °C**	**559.40 K**			
CSID	4444926	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	254.2375	**H bond donors**	2	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.44 g/cm^3
SMILES	O=C\1c3c(O/C(=C/1)c2ccccc2)cc(O)cc3O				
STD InChIKey	RTIXKCRFFJGDFG-UHFFFAOYAO				

Melting Points

mp °C	source
287.00	Alfa Aesar
285.50	PHYSPROP

cinchophen C16H11NO2[3, 64]



Compound Data

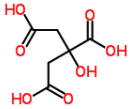
Melting point	**214.75 °C**	**487.90 K**			
CSID	8274	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	249.264	**H bond donors**	1	**ACD/LogP**	3.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	O=C(O)c1c3ccccc3nc(c1)c2ccccc2				
STD InChIKey	YTRMTPPVNRALON-UHFFFAOYAJ				

Melting Points

mp °C	source
215.00	Alfa Aesar
214.50	PHYSPROP

citric acid C6H8O7[3, 35, 35, 61, 64]

Compound Data



Melting point	**153.25 °C**	**426.40 K**			
CSID	305	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	192.1235	**H bond donors**	4	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.76 g/cm^3
SMILES	C(C(=O)O)C(CC(=O)O)(C(=O)O)O				
STD InChIKey	KRKNYBCHXYNGOX-UHFFFAOYAM				

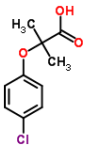
Melting Points

mp °C	source
154.00	Alfa Aesar
153.00	EPISuite-ChemSpider
153.00	Oxford University MSDS
153.00	PHYSPROP
	Values not used in calculating the average melting point
153.00	EPISuite-ChemSpider[1]

1. hydrate JCB

clofibric acid C10H11ClO3[3, 64]

Compound Data



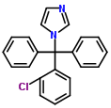
Melting point	**119.25 °C**	**392.40 K**			
CSID	2695	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.6455	**H bond donors**	1	**ACD/LogP**	2.72
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.26 g/cm^3
SMILES	Clc1ccc(OC(C(=O)O)(C)C)cc1				
STD InChIKey	TXCGAZHTZHNUAI-UHFFFAOYAP				

Melting Points

mp °C	source
120.00	Alfa Aesar
118.50	PHYSPROP

clotrimazole C22H17ClN2[9, 32, 48, 64]

Compound Data



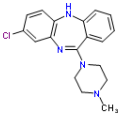
Melting point	**147.50 °C**	**420.65 K**			
CSID	2710	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	344.8368	**H bond donors**	0	**ACD/LogP**	5.44
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4				
STD InChIKey	VNFPBHJOKIVQEB-UHFFFAOYAO				

Melting Points

mp °C	source
147.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
148.00	DrugBank
147.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
148.00	PHYSPROP

clozapine C18H19ClN4[32, 44, 64]

Compound Data



Melting point	**183.63 °C**	**456.78 K**			
CSID	10442628	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	326.8233	**H bond donors**	1	**ACD/LogP**	3.94
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.32 g/cm^3
SMILES	CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl				
STD InChIKey	QZUDBNBUXVUHMW-UHFFFAOYAL				

Melting Points

mp °C	source
183.50	DrugBank

183.90	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
183.50	PHYSPROP

coronene C24H12[64, 70]

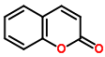
Compound Data

Melting point	**437.65 °C**	**710.80 K**			
CSID	8761	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	300.3521	**H bond donors**	0	**ACD/LogP**	7.11
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.47 g/cm^3
SMILES	c1cc2ccc3ccc4ccc5ccc6ccc1c7c2c3c4c5c67				
STD InChIKey	VPUGDVKSAQVFFS-UHFFFAOYAQ				

Melting Points

mp °C	source
437.30	PHYSPROP
438.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

coumarin C9H6O2[3, 64]



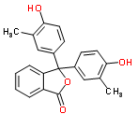
Compound Data

Melting point	**70.50 °C**	**343.65 K**			
CSID	13848793	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	146.1427	**H bond donors**	0	**ACD/LogP**	1.39
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	c1ccc2c(c1)ccc(=O)o2				
STD InChIKey	ZYGHJZDHTFUPRJ-UHFFFAOYAC				

Melting Points

mp °C	source
70.00	Alfa Aesar
71.00	PHYSPROP

cresolphthalein C22H18O4[3, 64]



Compound Data

Melting point	**223.50 °C**	**496.65 K**			
CSID	62217	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	346.3759	**H bond donors**	2	**ACD/LogP**	3.55
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.32 g/cm^3
SMILES	O=C1OC(c2ccccc12)(c3ccc(O)c(c3)C)c4ccc(O)c(c4)C				
STD InChIKey	CPBJMKMKNCRKQB-UHFFFAOYAJ				

Melting Points

mp °C	source
224.00	Alfa Aesar
223.00	PHYSPROP

cyanamide CH2N2[3, 61, 64]

Compound Data

Melting point	**44.85 °C**	**318.00 K**			
CSID	9480	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	42.04	**H bond donors**	2	**ACD/LogP**	-0.82
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	N#CN				
STD InChIKey	XZMCDFZZKTWFGF-UHFFFAOYAW				

Melting Points

mp °C	source
45.00	Alfa Aesar
44.00	Oxford University MSDS

45.56	PHYSPROP

cyanic iodide CIN[61, 64]

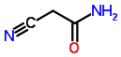
Compound Data

Melting point	**146.35 °C**	**419.50 K**			
CSID	10046	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	152.9219	**H bond donors**	0	**ACD/LogP**	1.33
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.67 g/cm^3
SMILES	IC#N				
STD InChIKey	WPBXOELOQKLBDF-UHFFFAOYAT				

Melting Points

mp °C	source
146.00	Oxford University MSDS
146.70	PHYSPROP

cyanoacetamide C3H4N2O[3, 48, 64]



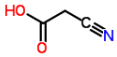
Compound Data

Melting point	**120.50 °C**	**393.65 K**			
CSID	7610	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	84.0767	**H bond donors**	2	**ACD/LogP**	-1.76
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.16 g/cm^3
SMILES	N#CCC(=O)N				
STD InChIKey	DGJMPUGMZIKDRO-UHFFFAOYAB				

Melting Points

mp °C	source
120.00	Alfa Aesar
120.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
121.50	PHYSPROP

cyanoacetic acid C3H3NO2[3, 64]



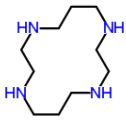
Compound Data

Melting point	**66.50 °C**	**339.65 K**			
CSID	9357	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	85.0614	**H bond donors**	1	**ACD/LogP**	-0.76
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	N#CCC(=O)O				
STD InChIKey	MLIREBYILWEBDM-UHFFFAOYAD				

Melting Points

mp °C	source
67.00	Alfa Aesar
66.00	PHYSPROP

cyclam C10H24N4[3, 64]



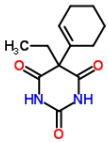
Compound Data

Melting point	**185.50 °C**	**458.65 K**			
CSID	58489	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	200.3244	**H bond donors**	4	**ACD/LogP**	-0.97
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.86 g/cm^3
SMILES	N1CCNCCCNCCNCCC1				
STD InChIKey	MDAXKAUIABOHTD-UHFFFAOYAV				

Melting Points

mp °C	source
186.00	Alfa Aesar
185.00	PHYSPROP

cyclobarbital C12H16N2O3[44, 64]



Compound Data

Melting point	**172.75 °C**	**445.90 K**			
CSID	5632	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	236.267	**H bond donors**	2	**ACD/LogP**	1.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(/C2=C/CCCC2)CC				
STD InChIKey	WTYGAUXICFETTC-UHFFFAOYAC				

Melting Points

mp °C	source
172.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
173.00	PHYSPROP

cyclobutane C4H8[4, 25, 64]

Compound Data

Melting point	**-90.76 °C**	**182.39 K**			
CSID	8894	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	56.1063	**H bond donors**	0	**ACD/LogP**	2.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CCC1				
STD InChIKey	PMPVIKIVABFJJI-UHFFFAOYAP				

Melting Points

mp °C	source
-91.00	American Petroleum Institute. Research Project 44; Selected ...
-90.67	Cheric
-90.60	PHYSPROP

cyclobutanone C4H6O[3, 64, 66]

Compound Data

Melting point	**-51.30 °C**	**221.85 K**			
CSID	13840	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	70.0898	**H bond donors**	0	**ACD/LogP**	-0.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.04 g/cm^3
SMILES	O=C1CCC1				
STD InChIKey	SHQSVMDWKBRBGB-UHFFFAOYAY				

Melting Points

mp °C	source
-51.00	Alfa Aesar
-50.90	PHYSPROP
-52.00	R. Arndt; Hs. H. Gunthard;T. Gaumann T Helvetica Chimica Act...

cyclobutylmethane C5H10[52, 64]

Compound Data

Melting point	**-161.50 °C**	**111.64 K**			
CSID	11232	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3
SMILES	CC1CCC1				
STD InChIKey	BDJAEZRIGNCQBZ-UHFFFAOYAR				

Melting Points

mp °C	source
-161.51	Lemaire HP; Livingston RL. Journal of the American Chemical ...
-161.50	PHYSPROP

cyclodecanol C10H20O[47, 64]

Compound Data

Melting point	**40.17 °C**	**313.32 K**			
CSID	14436	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	156.2652	**H bond donors**	1	**ACD/LogP**	3.60
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.90 g/cm^3
SMILES	OC1CCCCCCCCC1				
STD InChIKey	WFRBMXFCEAHLGH-UHFFFAOYAJ				

Melting Points

mp °C	source
39.85	IUCr
40.50	PHYSPROP

cyclodecanone C10H18O[2, 64]

Compound Data

Melting point	**26.00 °C**	**299.15 K**			
CSID	66551	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	154.2493	**H bond donors**	0	**ACD/LogP**	3.02
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.89 g/cm^3
SMILES	O=C1CCCCCCCCC1				
STD InChIKey	SXOZDDAFVJANJP-UHFFFAOYAD				

Melting Points

mp °C	source
24.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
28.00	PHYSPROP

cyclododecane C12H24[4, 61, 64, 64]

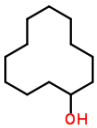
Compound Data

Melting point	**60.35 °C**	**333.50 K**			
CSID	8911	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	168.319	**H bond donors**	0	**ACD/LogP**	6.33
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CCCCCCCCCCC1				
STD InChIKey	DDTBPAQBQHZRDW-UHFFFAOYAN				

Melting Points

mp °C	source
61.00	American Petroleum Institute. Research Project 44; Selected ...
61.00	Oxford University MSDS
60.40	PHYSPROP
59.00	PHYSPROP

cyclododecanol C12H24O[2, 3, 64]



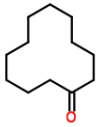
Compound Data

Melting point	**77.17 °C**	**350.32 K**			
CSID	14836	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.3184	**H bond donors**	1	**ACD/LogP**	4.73
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.88 g/cm^3
SMILES	OC1CCCCCCCCCCC1				
STD InChIKey	SFVWPXMPRCIVOK-UHFFFAOYAM				

Melting Points

mp °C	source
76.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
78.00	Alfa Aesar
77.50	PHYSPROP

cyclododecanone C12H22O[2, 3]



Compound Data

Melting point	**60.50 °C**	**333.65 K**			
CSID	12690	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.3025	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	O=C1CCCCCCCCCCC1				
STD InChIKey	SXVPOSFURRDKBO-UHFFFAOYAN				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
61.00	Alfa Aesar

cycloheptatriene C7H8[3, 64]

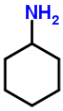
Compound Data

Melting point	**-79.75 °C**	**193.40 K**			
CSID	10534	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	92.1384	**H bond donors**	0	**ACD/LogP**	2.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.89 g/cm^3
SMILES	C1=C\C/C=C\C=C1				
STD InChIKey	CHVJITGCYZJHLR-UHFFFAOYAI				

Melting Points

mp °C	source
-80.00	Alfa Aesar
-79.50	PHYSPROP

cyclohexanamine C6H13N[2, 3, 35, 61, 64]



Compound Data

Melting point	**-17.68 °C**	**255.47 K**			
CSID	7677	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	99.1741	**H bond donors**	2	**ACD/LogP**	1.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	NC1CCCCC1				
STD InChIKey	PAFZNILMFXTMIY-UHFFFAOYAP				

Melting Points

mp °C	source
-17.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-18.00	Alfa Aesar
-17.70	EPISuite-ChemSpider
-18.00	Oxford University MSDS
-17.70	PHYSPROP

cyclohexane C6H12[3, 4, 59, 61, 64]

Compound Data

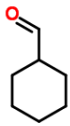
Melting point	**6.81 °C**	**279.96 K**			
CSID	7787	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CCCCC1				
STD InChIKey	XDTMQSROBMDMFD-UHFFFAOYAZ				

Melting Points

mp °C	source
7.00	Alfa Aesar

7.00	American Petroleum Institute. Research Project 44; Selected ...
6.45	NIST Web Book
7.00	Oxford University MSDS
6.60	PHYSPROP

cyclohexanecarbaldehyde C7H12O[3, 3]



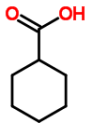
Compound Data

Melting point	**34.75 °C**	**307.90 K**			
CSID	15443	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	112.1696	**H bond donors**	0	**ACD/LogP**	1.90
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.99 g/cm^3
SMILES	O=CC1CCCCC1				
STD InChIKey	KVFDZFBHBWTVID-UHFFFAOYAG				

Melting Points

mp °C	source
34.50	Alfa Aesar
35.00	Alfa Aesar

cyclohexanecarboxylic acid C7H12O2[3, 35, 42, 64]



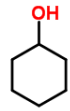
Compound Data

Melting point	**31.00 °C**	**304.15 K**			
CSID	7135	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.169	**H bond donors**	1	**ACD/LogP**	1.77
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	O=C(O)C1CCCCC1				
STD InChIKey	NZNMSOFKMUBTKW-UHFFFAOYAH				

Melting Points

mp °C	source
31.00	Alfa Aesar
31.50	EPISuite-ChemSpider
30.00	GoodScents
31.50	PHYSPROP

cyclohexanol C6H12O[2, 3, 28, 61, 64]



Compound Data

Melting point	**23.47 °C**	**296.62 K**			
CSID	7678	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	100.1589	**H bond donors**	1	**ACD/LogP**	1.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	C1CCC(CC1)O				
STD InChIKey	HPXRVTGHNJAIIH-UHFFFAOYAN				

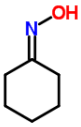
Melting Points

mp °C	source
21.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
24.00	Alfa Aesar
25.93	CRC Handbook of Chemistry and Physics
21.00	Oxford University MSDS
25.40	PHYSPROP

cyclohexanone oxime C6H11NO[3, 48, 61, 64]

Compound Data

Melting point	**89.50 °C**	**362.65 K**			
CSID	7236	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	113.1576	**H bond donors**	1	**ACD/LogP**	1.12
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	3



1.10 g/cm

SMILES	O\N=C1\CCCCC1
STD InChIKey	VEZUQRBDRNJBJY-UHFFFAOYAH

Melting Points

mp °C	source
89.00	Alfa Aesar
89.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
90.00	Oxford University MSDS
90.00	PHYSPROP

cyclohexene C6H10[3, 4, 61, 64]

Compound Data

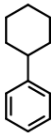
Melting point	**-103.88 °C**	**169.27 K**			
CSID	7788	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.92
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.82 g/cm^3
SMILES	C1CCC=CC1				
STD InChIKey	HGCIXCUEYOPUTN-UHFFFAOYAQ				

Melting Points

mp °C	source
-104.00	Alfa Aesar
-104.00	American Petroleum Institute. Research Project 44; Selected ...
-104.00	Oxford University MSDS
-103.50	PHYSPROP

cyclohexylbenzene C12H16[2, 3, 61, 64]

Compound Data



Melting point	**5.83 °C**	**278.97 K**			
CSID	12674	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	160.2554	**H bond donors**	0	**ACD/LogP**	4.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.94 g/cm^3
SMILES	c1cc(ccc1)C2CCCCC2				
STD InChIKey	IGARGHRYKHJQSM-UHFFFAOYAC				

Melting Points

mp °C	source
5.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
6.00	Alfa Aesar
5.00	Oxford University MSDS
7.30	PHYSPROP

cyclooctane C8H16[3, 4, 64]

Compound Data

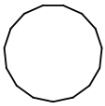
Melting point	**13.93 °C**	**287.08 K**			
CSID	8909	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.22
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CCCCCCC1				
STD InChIKey	WJTCGQSWYFHTAC-UHFFFAOYAO				

Melting Points

mp °C	source
12.00	Alfa Aesar
15.00	American Petroleum Institute. Research Project 44; Selected ...

14.80	PHYSPROP

cyclopentadecane $C_{15}H_{30}$[4, 64]



Compound Data

Melting point	**61.65 °C**	**334.80 K**			
CSID	60848	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	210.3987	**H bond donors**	0	**ACD/LogP**	8.46
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CCCCCCCCCCCCCC1				
STD InChIKey	SRONXYPFSAKOGH-UHFFFAOYAZ				

Melting Points

mp °C	source
62.00	American Petroleum Institute. Research Project 44; Selected ...
61.30	PHYSPROP

cyclopentane C_5H_{10}[3, 4, 59, 61, 64]

Compound Data

Melting point	**-93.95 °C**	**179.20 K**			
CSID	8896	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.82
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CCCC1				
STD InChIKey	RGSFGYAAUTVSQA-UHFFFAOYAL				

Melting Points

mp °C	source
-94.00	Alfa Aesar
-94.00	American Petroleum Institute. Research Project 44; Selected ...
-93.95	NIST Web Book
-94.00	Oxford University MSDS
-93.80	PHYSPROP

cyclopentanol $C_5H_{10}O$[2, 3, 28, 61, 62, 64, 79]

Compound Data

Melting point	**-18.54 °C**	**254.61 K**			
CSID	7026	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	86.1323	**H bond donors**	1	**ACD/LogP**	0.76
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	C1CCC(C1)O				
STD InChIKey	XCIXKGXIYUWCLL-UHFFFAOYAS				

Melting Points

mp °C	source
-19.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-19.00	Alfa Aesar
-17.50	CRC Handbook of Chemistry and Physics
-19.00	Oxford University MSDS
-16.25	Parks GS; Kennedy WD; Gates RR; Mosley JR; Moore GE; Renquis...
-19.00	PHYSPROP
-20.00	White AH; Bishop WS Journal of the American Chemical Society...

cyclopentanone C_5H_8O[2, 3, 28, 61, 64]

Compound Data

Melting point	**-51.24 °C**	**221.91 K**			
CSID	8141	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	84.1164	**H bond donors**	0	**ACD/LogP**	0.29
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	3

0.99 g/cm

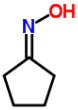
SMILES	C1CCC(=O)C1
STD InChIKey	BGTOWKSIORTVQH-UHFFFAOYAP

Melting Points

mp °C	source
-51.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-51.00	Alfa Aesar
-51.90	CRC Handbook of Chemistry and Physics
-51.00	Oxford University MSDS
-51.30	PHYSPROP

cyclopentanone oxime C5H9NO[3, 64]

Compound Data



Melting point	**56.90 °C 330.05 K**				
CSID	13844	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	99.1311	**H bond donors**	1	**ACD/LogP**	0.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.15 g/cm^3
SMILES	O\N=C1/CCCC1				
STD InChIKey	YGNXYFLJZILPEK-UHFFFAOYAT				

Melting Points

mp °C	source
56.00	Alfa Aesar
57.80	PHYSPROP

cyclopentene C5H8[3, 4, 61, 64]

Compound Data

Melting point	**-135.03 °C 138.12 K**				
CSID	8544	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	68.117	**H bond donors**	0	**ACD/LogP**	2.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.83 g/cm^3
SMILES	C1CC=CC1				
STD InChIKey	LPIQUOYDBNQMRZ-UHFFFAOYAS				

Melting Points

mp °C	source
-135.00	Alfa Aesar
-135.00	American Petroleum Institute. Research Project 44; Selected ...
-135.00	Oxford University MSDS
-135.10	PHYSPROP

cyclopentylamine C5H11N[3, 57, 64]

Compound Data

Melting point	**-84.47 °C 188.68 K**				
CSID	2803	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	85.1475	**H bond donors**	2	**ACD/LogP**	0.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.88 g/cm^3
SMILES	NC1CCCC1				
STD InChIKey	NISGSNTVMOOSJQ-UHFFFAOYAM				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-85.70	Mme M. L. Labruyere-Verhavert. Bulletin des Societes Chimiqu...
-82.70	PHYSPROP

cyclopropane C3H6[59, 64, 68]

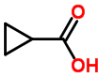
Compound Data

Melting point	**-127.37 °C**	**145.78 K**			
CSID	6111	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	42.0797	**H bond donors**	0	**ACD/LogP**	1.58
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.79 g/cm^3
SMILES	C1CC1				
STD InChIKey	LVZWSLJZHVFIQJ-UHFFFAOYAL				

Melting Points

mp °C	source
-127.15	NIST Web Book
-127.40	PHYSPROP
-127.56	Ruehrwein RA; Powell TM. Journal of the American Chemical So...

cyclopropanecarboxylic acid C4H6O2[17, 19, 24, 64, 74]



Compound Data

Melting point	**17.45 °C**	**290.60 K**			
CSID	14890	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	86.0892	**H bond donors**	1	**ACD/LogP**	0.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.31 g/cm^3
SMILES	O=C(O)C1CC1				
STD InChIKey	YMGUBTXCNDTFJI-UHFFFAOYAF				

Melting Points

mp °C	source
18.00	ChemBlink
15.50	Chemical Book
18.50	Chemyq
18.50	PHYSPROP
16.75	Subbotin OA; Kozmin AS; Grishin YuK; Sergeyev NM; Bolesov IG...
	Values not used in calculating the average melting point
5.00	Alfa Aesar[1]

1. clearly out of range JCB

cyclopropylmethane C4H8[43, 59, 64]

Compound Data

Melting point	**-177.24 °C**	**95.91 K**			
CSID	11167	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	56.1063	**H bond donors**	0	**ACD/LogP**	2.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3
SMILES	CC1CC1				
STD InChIKey	VNXBKJFUJUWOCW-UHFFFAOYAC				

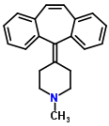
Melting Points

mp °C	source
-177.16	Gragson JT; Greenlee KW; Derfer JM; Boord CE. Journal of the...
-177.25	NIST Web Book
-177.30	PHYSPROP

cyproheptadine C21H21N[44, 59, 64]

Compound Data

Melting point	**112.37 °C**	**385.52 K**			
CSID	2810	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	287.3981	**H bond donors**	0	**ACD/LogP**	6.41
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c43\C(=C1/CCN(C)CC1)c2ccccc2\C=C/c3cccc4				



STD InChIKey	JJCFRYNCJDLXIK-UHFFFAOYAW

Melting Points

mp °C	source
112.80	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
111.50	NIST Web Book
112.80	PHYSPROP
	Values not used in calculating the average melting point
216.00	DrugBank[1]

1. HCl salt JCB

dabco C6H12N2[3, 64]

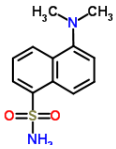
Compound Data

Melting point	**158.50 °C**	**431.65 K**			
CSID	8882	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	112.1729	**H bond donors**	0	**ACD/LogP**	-0.85
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	N12CCN(CC1)CC2				
STD InChIKey	IMNIMPAHZVJRPE-UHFFFAOYAP				

Melting Points

mp °C	source
158.00	Alfa Aesar
159.00	PHYSPROP

dansyl amide C12H14N2O2S[3, 64]



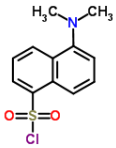
Compound Data

Melting point	**219.75 °C**	**492.90 K**			
CSID	58587	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	250.3168	**H bond donors**	2	**ACD/LogP**	2.01
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=S(=O)(c1cccc2c1cccc2N(C)C)N				
STD InChIKey	TYNBFJJKZPTRKS-UHFFFAOYAD				

Melting Points

mp °C	source
220.00	Alfa Aesar
219.50	PHYSPROP

dansyl chloride C12H12ClNO2S[3, 64]



Compound Data

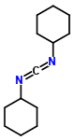
Melting point	**71.00 °C**	**344.15 K**			
CSID	11308	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	269.7472	**H bond donors**	0	**ACD/LogP**	3.67
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.36 g/cm^3
SMILES	ClS(=O)(=O)c1cccc2c1cccc2N(C)C				
STD InChIKey	XPDXVDYUQZHFPV-UHFFFAOYAI				

Melting Points

mp °C	source
72.00	Alfa Aesar
70.00	PHYSPROP

DCC C13H22N2[3, 3, 19, 55, 64, 72, 84]

Compound Data



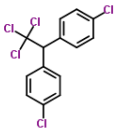
Melting point	**35.11 °C**	**308.26 K**			
CSID	10408	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	206.3272	**H bond donors**	0	**ACD/LogP**	5.54
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	N(=C=N\C1CCCCC1)\C2CCCCC2				
STD InChIKey	QOSSAOTZNIDXMA-UHFFFAOYAO				

Melting Points

mp °C	source
35.00	Alfa Aesar
34.50	Alfa Aesar
34.50	Chemical Book
35.50	Merck Chemicals
34.50	PHYSPROP
35.75	Sigma-Aldrich
36.00	Wolfram Alpha

DDT C14H9Cl5[27, 58, 61, 61, 64, 65, 70, 70, 80]

Compound Data



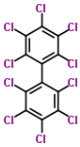
Melting point	**108.67 °C**	**381.82 K**			
CSID	2928	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	354.4863	**H bond donors**	0	**ACD/LogP**	5.92
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.45 g/cm^3
SMILES	Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl				
STD InChIKey	YVGGHNCTFXOJCH-UHFFFAOYAJ				

Melting Points

mp °C	source
108.75	Cornell
108.30	NIOSH
108.50	Oxford University MSDS
108.50	Oxford University MSDS
108.50	PHYSPROP
108.75	PiedPiper
109.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
109.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
108.75	WHO

decachlorobiphenyl C12Cl10[64, 70]

Compound Data



Melting point	**305.90 °C**	**579.05 K**			
CSID	15484	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	498.6584	**H bond donors**	0	**ACD/LogP**	8.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.82 g/cm^3
SMILES	Clc1c(c(Cl)c(Cl)c(Cl)c1Cl)c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl				
STD InChIKey	ONXPZLFXDMAPRO-UHFFFAOYAX				

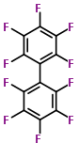
Melting Points

mp °C	source
305.80	PHYSPROP
306.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

decafluorobiphenyl C12F10[3, 61, 64]

Compound Data

Melting point	**67.50 °C**	**340.65 K**			
CSID	61266	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	334.1124	**H bond donors**	0	**ACD/LogP**	6.73



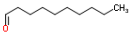
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.70 g/cm^3
SMILES	Fc1c(c(F)c(F)c(F)c1F)c2c(F)c(F)c(F)c(F)c2F				
STD InChIKey	ONUFSRWQCKNVSL-UHFFFAOYAP				

Melting Points

mp °C	source
68.00	Alfa Aesar
67.00	Oxford University MSDS
67.50	PHYSPROP

decanal C10H20O[3, 4, 64]

Compound Data



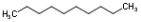
Melting point	**-5.33 °C**	**267.82 K**			
CSID	7883	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	156.2652	**H bond donors**	0	**ACD/LogP**	4.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.82 g/cm^3
SMILES	O=CCCCCCCCCC				
STD InChIKey	KSMVZQYAVGTKIV-UHFFFAOYAQ				

Melting Points

mp °C	source
-5.00	Alfa Aesar
-6.00	American Petroleum Institute. Research Project 44; Selected ...
-5.00	PHYSPROP

decane C10H22[3, 4, 32, 59, 61, 64]

Compound Data



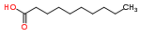
Melting point	**-29.88 °C**	**243.27 K**			
CSID	14840	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	142.2817	**H bond donors**	0	**ACD/LogP**	5.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.73 g/cm^3
SMILES	CCCCCCCCCC				
STD InChIKey	DIOQZVSQGTUSAI-UHFFFAOYAR				

Melting Points

mp °C	source
-30.00	Alfa Aesar
-30.00	American Petroleum Institute. Research Project 44; Selected ...
-29.70	DrugBank
-29.85	NIST Web Book
-30.00	Oxford University MSDS
-29.70	PHYSPROP

decanoic acid C10H20O2[3, 4, 61, 61, 64]

Compound Data



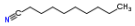
Melting point	**31.38 °C**	**304.53 K**			
CSID	2863	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.2646	**H bond donors**	1	**ACD/LogP**	3.96
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	0.92 g/cm^3
SMILES	O=C(O)CCCCCCCCC				
STD InChIKey	GHVNFZFCNZKVNT-UHFFFAOYAC				

Melting Points

mp °C	source
31.00	Alfa Aesar
32.00	American Petroleum Institute. Research Project 44; Selected ...

31.00	Oxford University MSDS
31.00	Oxford University MSDS
31.90	PHYSPROP

decanonitrile C10H19N[3, 31, 64]



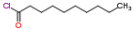
Compound Data

Melting point	**-15.97 °C**	**257.18 K**			
CSID	67360	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	153.2646	**H bond donors**	0	**ACD/LogP**	3.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.82 g/cm^3
SMILES	N#CCCCCCCCCC				
STD InChIKey	HBZDPWBWBJMYRY-UHFFFAOYAE				

Melting Points

mp °C	source
-15.00	Alfa Aesar
-15.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-17.90	PHYSPROP

decanoyl chloride C10H19ClO[3, 64]



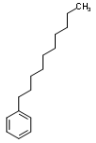
Compound Data

Melting point	**-34.75 °C**	**238.40 K**			
CSID	60340	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	190.7103	**H bond donors**	0	**ACD/LogP**	4.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.94 g/cm^3
SMILES	ClC(=O)CCCCCCCCC				
STD InChIKey	IPIVAXLHTVNRBS-UHFFFAOYAH				

Melting Points

mp °C	source
-35.00	Alfa Aesar
-34.50	PHYSPROP

decylbenzene C16H26[4, 61, 64]



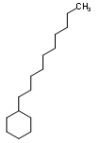
Compound Data

Melting point	**-14.13 °C**	**259.02 K**			
CSID	7430	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	218.3776	**H bond donors**	0	**ACD/LogP**	7.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.86 g/cm^3
SMILES	c1ccccc1CCCCCCCCCC				
STD InChIKey	UZILCZKGXMQEQR-UHFFFAOYAU				

Melting Points

mp °C	source
-14.00	American Petroleum Institute. Research Project 44; Selected ...
-14.00	Oxford University MSDS
-14.40	PHYSPROP

decylcyclohexane C16H32[4, 64]



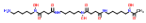
Compound Data

Melting point	**-1.85 °C**	**271.30 K**			
CSID	14942	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	224.4253	**H bond donors**	0	**ACD/LogP**	8.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.81 g/cm^3
SMILES	C(CCC1CCCCC1)CCCCCCC				
STD InChIKey	STWFZICHPLEOIC-UHFFFAOYAF				

Melting Points

mp °C	source
-2.00	American Petroleum Institute. Research Project 44; Selected ...
-1.70	PHYSPROP

deferoxamine C25H48N6O8[32, 64]



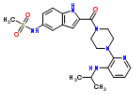
Compound Data

Melting point	**139.50 °C**	**412.65 K**			
CSID	2867	**H bond acceptors**	14	**Rule of 5 violations**	3
Molecular weight	560.684	**H bond donors**	7	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	27	**Predicted density**	1.21 g/cm^3
SMILES	CC(=O)N(CCCCCNC(=O)CCC(=O)N(CCCCCNC(=O)CCC(=O)N(CCCCCN)O)O)O				
STD InChIKey	UBQYURCVBFRUQT-UHFFFAOYAW				

Melting Points

mp °C	source
139.00	DrugBank
140.00	PHYSPROP

delavirdine C22H28N6O3S[9, 32]



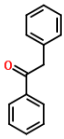
Compound Data

Melting point	**226.50 °C**	**499.65 K**			
CSID	5423	**H bond acceptors**	9	**Rule of 5 violations**	0
Molecular weight	456.5611	**H bond donors**	3	**ACD/LogP**	-0.84
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.39 g/cm^3
SMILES	O=S(=O)(Nc1cc2cc(nc2cc1)C(=O)N4CCN(c3ncccc3NC(C)C)CC4)C				
STD InChIKey	WHBIGIKBNXZKFE-UHFFFAOYAY				

Melting Points

mp °C	source
226.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
227.00	DrugBank

deoxybenzoin C14H12O[3, 64]



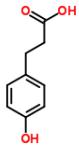
Compound Data

Melting point	**57.50 °C**	**330.65 K**			
CSID	9554	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	196.2445	**H bond donors**	0	**ACD/LogP**	3.18
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.08 g/cm^3
SMILES	O=C(c1ccccc1)Cc2ccccc2				
STD InChIKey	OTKCEEWUXHVZQI-UHFFFAOYAG				

Melting Points

mp °C	source
55.00	Alfa Aesar
60.00	PHYSPROP

desaminotyrosine C9H10O3[3, 48, 64]



Compound Data

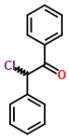
Melting point	**129.93 °C**	**403.08 K**			
CSID	9965	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	2	**ACD/LogP**	1.10
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.26 g/cm^3
SMILES	O=C(O)CCc1ccc(O)cc1				
STD InChIKey	NMHMNPHRMNGLLB-UHFFFAOYAT				

Melting Points

mp °C	source
129.00	Alfa Aesar

130.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
130.80	PHYSPROP

desyl chloride C14H11ClO[3, 64]



Compound Data

Melting point	**67.75 °C**	**340.90 K**			
CSID	86040	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	230.6895	**H bond donors**	0	**ACD/LogP**	3.30
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.19 g/cm^3
SMILES	ClC(C(=O)c1ccccc1)c2ccccc2				
STD InChIKey	RXDYOLRABMJTEF-UHFFFAOYAQ				

Melting Points

mp °C	source
67.00	Alfa Aesar
68.50	PHYSPROP

di-butyl sebacate C18H34O4[3, 64]

Compound Data

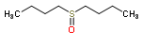
Melting point	**-10.50 °C**	**262.65 K**			
CSID	13837584	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	314.4602	**H bond donors**	0	**ACD/LogP**	5.97
Phase 25 °C	liquid/gas	**Rotatable bonds**	17	**Predicted density**	0.94 g/cm^3
SMILES	CCCCOC(=O)CCCCCCCCC(=O)OCCCC				
STD InChIKey	PYGXAGIECVVIOZ-UHFFFAOYAE				

Melting Points

mp °C	source
-11.00	Alfa Aesar
-10.00	PHYSPROP

di-n-butyl sulfoxide C8H18OS[3, 64]

Compound Data



Melting point	**32.80 °C**	**305.95 K**			
CSID	15708	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.2929	**H bond donors**	0	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	0.95 g/cm^3
SMILES	O=S(CCCC)CCCC				
STD InChIKey	LOWMYOWHQMKBTM-UHFFFAOYAX				

Melting Points

mp °C	source
33.00	Alfa Aesar
32.60	PHYSPROP

di-n-pentyl sulfide C10H22S[3, 64]

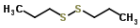
Compound Data

Melting point	**-51.15 °C**	**222.00 K**			
CSID	12810	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	174.3467	**H bond donors**	0	**ACD/LogP**	5.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.84 g/cm^3
SMILES	S(CCCCC)CCCCC				
STD InChIKey	JOZDADPMWLVEJK-UHFFFAOYAV				

Melting Points

mp °C	source
-51.00	Alfa Aesar
-51.30	PHYSPROP

di-n-propyl disulfide C6H14S2[3, 64]



Compound Data

Melting point	**-85.80 °C**	**187.35 K**			
CSID	11871	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	150.3054	**H bond donors**	0	**ACD/LogP**	3.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.97 g/cm^3
SMILES	S(SCCC)CCC				
STD InChIKey	ALVPFGSHPUPROW-UHFFFAOYAZ				

Melting Points

mp °C	source
-86.00	Alfa Aesar
-85.60	PHYSPROP

di-n-propyl sulfide C6H14S[3, 4, 64]

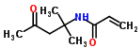
Compound Data

Melting point	**-102.50 °C**	**170.65 K**			
CSID	7827	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.2404	**H bond donors**	0	**ACD/LogP**	3.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.83 g/cm^3
SMILES	S(CCC)CCC				
STD InChIKey	ZERULLAPCVRMCO-UHFFFAOYAQ				

Melting Points

mp °C	source
-102.00	Alfa Aesar
-103.00	American Petroleum Institute. Research Project 44; Selected ...
-102.50	PHYSPROP

diacetone acrylamide C9H15NO2[3, 64]



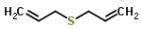
Compound Data

Melting point	**56.25 °C**	**329.40 K**			
CSID	16896	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	169.2209	**H bond donors**	1	**ACD/LogP**	-0.05
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.96 g/cm^3
SMILES	O=C(CC(NC(=O)\C=C)(C)C)C				
STD InChIKey	OMNKZBIFPJNNIO-UHFFFAOYAV				

Melting Points

mp °C	source
55.00	Alfa Aesar
57.50	PHYSPROP

diallyl sulfide C6H10S[3, 64]



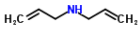
Compound Data

Melting point	**-84.00 °C**	**189.15 K**			
CSID	11128	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	114.2086	**H bond donors**	0	**ACD/LogP**	2.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.87 g/cm^3
SMILES	S(C\C=C)C\C=C				
STD InChIKey	UBJVUCKUDDKUJF-UHFFFAOYAC				

Melting Points

mp °C	source
-83.00	Alfa Aesar
-85.00	PHYSPROP

diallylamine C6H11N[3, 64]



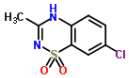
Compound Data

Melting point	**-88.20 °C**	**184.95 K**			
CSID	21106561	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	97.1582	**H bond donors**	1	**ACD/LogP**	1.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.77 g/cm^3
SMILES	C=CCNCC=C				
STD InChIKey	DYUWTXWIYMHBQS-UHFFFAOYAO				

Melting Points

mp °C	source
-88.00	Alfa Aesar
-88.40	PHYSPROP

diazoxide C8H7ClN2O2S[32, 44, 64]



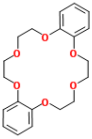
Compound Data

Melting point	**329.40 °C**	**602.55 K**			
CSID	2911	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	230.6714	**H bond donors**	1	**ACD/LogP**	1.07
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.61 g/cm^3
SMILES	Clc1ccc2c(c1)S(=O)(=O)/N=C(\N2)C				
STD InChIKey	GDLBFKVLRPITMI-UHFFFAOYAC				

Melting Points

mp °C	source
330.50	DrugBank
327.20	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
330.50	PHYSPROP

dibenzo-18-crown-6 C20H24O6[3, 64]



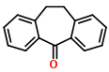
Compound Data

Melting point	**162.50 °C**	**435.65 K**			
CSID	24722	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	360.401	**H bond donors**	0	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	O1c3c(OCCOCCOc2ccccc2OCCOCC1)cccc3				
STD InChIKey	YSSSPARMOAYJTE-UHFFFAOYAB				

Melting Points

mp °C	source
162.00	Alfa Aesar
163.00	PHYSPROP

dibenzosuberone C15H12O[3, 64]



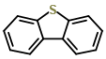
Compound Data

Melting point	**31.50 °C**	**304.65 K**			
CSID	13927	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	208.2552	**H bond donors**	0	**ACD/LogP**	4.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	O=C2c1c(cccc1)CCc3c2cccc3				
STD InChIKey	BMVWCPGVLSILMU-UHFFFAOYAF				

Melting Points

mp °C	source
33.00	Alfa Aesar
30.00	PHYSPROP

dibenzothiophene C12H8S[3, 64]



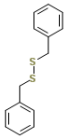
Compound Data

Melting point	**98.00 °C**	**371.15 K**			
CSID	2915	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	184.2569	**H bond donors**	0	**ACD/LogP**	4.49
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	c1ccc2c(c1)c3ccccc3s2				
STD InChIKey	IYYZUPMFVPLQIF-UHFFFAOYAY				

Melting Points

mp °C	source
99.00	Alfa Aesar
97.00	PHYSPROP

dibenzyl disulfide C14H14S2[3, 64]



Compound Data

Melting point	**70.75 °C**	**343.90 K**			
CSID	8662	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	246.391	**H bond donors**	0	**ACD/LogP**	5.35
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.17 g/cm^3
SMILES	S(SCc1ccccc1)Cc2ccccc2				
STD InChIKey	GVPWHKZIJBODOX-UHFFFAOYAF				

Melting Points

mp °C	source
70.00	Alfa Aesar
71.50	PHYSPROP

dibenzyl ether C14H14O[2, 3, 64]

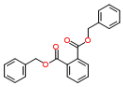
Compound Data

Melting point	**3.53 °C**	**276.68 K**			
CSID	21105876	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	198.2604	**H bond donors**	0	**ACD/LogP**	3.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.05 g/cm^3
SMILES	c1ccc(cc1)COCc2ccccc2				
STD InChIKey	MHDVGSVTJDSBDK-UHFFFAOYAM				

Melting Points

mp °C	source
3.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
4.00	Alfa Aesar
3.60	PHYSPROP

dibenzyl phthalate C22H18O4[3, 64]



Compound Data

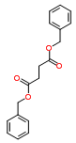
Melting point	**42.50 °C**	**315.65 K**			
CSID	191496	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	346.3759	**H bond donors**	0	**ACD/LogP**	5.18
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.21 g/cm^3
SMILES	O=C(OCc1ccccc1)c3ccccc3C(=O)OCc2ccccc2				
STD InChIKey	UCVPKAZCQPRWAY-UHFFFAOYAQ				

Melting Points

mp °C	source
41.00	Alfa Aesar
44.00	PHYSPROP

dibenzyl succinate C18H18O4[3, 64]

Compound Data



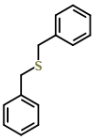
Melting point	**47.25 °C**	**320.40 K**			
CSID	7370	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	298.3331	**H bond donors**	0	**ACD/LogP**	3.70
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OCc1ccccc1)CCC(=O)OCc2ccccc2				
STD InChIKey	ODBOBZHTGBGYCK-UHFFFAOYAQ				

Melting Points

mp °C	source
45.00	Alfa Aesar
49.50	PHYSPROP

dibenzyl sulfide C14H14S[3, 64]

Compound Data



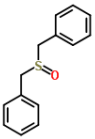
Melting point	**49.25 °C**	**322.40 K**			
CSID	10407	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	214.326	**H bond donors**	0	**ACD/LogP**	4.19
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	S(Cc1ccccc1)Cc2ccccc2				
STD InChIKey	LUFPJJNWMYZRQE-UHFFFAOYAV				

Melting Points

mp °C	source
49.00	Alfa Aesar
49.50	PHYSPROP

dibenzyl sulfoxide C14H14OS[48, 64]

Compound Data



Melting point	**133.50 °C**	**406.65 K**			
CSID	11618	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	230.3254	**H bond donors**	0	**ACD/LogP**	1.99
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	O=S(Cc1ccccc1)Cc2ccccc2				
STD InChIKey	HTMQZWFSTJVJEQ-UHFFFAOYAR				

Melting Points

mp °C	source
133.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
134.00	PHYSPROP

dibromochloromethane CHBr2Cl[2, 3, 64]

Compound Data

Melting point	**-21.33 °C**	**251.82 K**			
CSID	29036	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	208.2796	**H bond donors**	0	**ACD/LogP**	2.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.50 g/cm^3
SMILES	BrC(Br)Cl				
STD InChIKey	GATVIKZLVQHOMN-UHFFFAOYAQ				

Melting Points

mp °C	source
-22.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-22.00	Alfa Aesar
-20.00	PHYSPROP

dibromomethane CH2Br2[3, 31, 61, 64]

Compound Data

Melting point	**-52.62 °C**	**220.52 K**

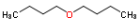
CSID	2916	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	173.8346	**H bond donors**	0	**ACD/LogP**	1.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.43 g/cm^3
SMILES	BrCBr				
STD InChIKey	FJBFPHVGVWTDIP-UHFFFAOYAK				

Melting Points

mp °C	source
-53.00	Alfa Aesar
-53.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-52.00	Oxford University MSDS
-52.50	PHYSPROP

dibutyl ether C8H18O[2, 3, 61, 64]

Compound Data



Melting point	**-96.52 °C**	**176.62 K**			
CSID	8569	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	130.2279	**H bond donors**	0	**ACD/LogP**	3.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.78 g/cm^3
SMILES	O(CCCC)CCCC				
STD InChIKey	DURPTKYDGMDSBL-UHFFFAOYAH				

Melting Points

mp °C	source
-98.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-95.00	Alfa Aesar
-97.90	Oxford University MSDS
-95.20	PHYSPROP

dibutyl sulfide C8H18S[3, 61, 64]

Compound Data

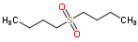
Melting point	**-79.90 °C**	**193.25 K**			
CSID	10536	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	146.2935	**H bond donors**	0	**ACD/LogP**	4.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.84 g/cm^3
SMILES	S(CCCC)CCCC				
STD InChIKey	HTIRHQRTDBPHNZ-UHFFFAOYAZ				

Melting Points

mp °C	source
-80.00	Alfa Aesar
-80.00	Oxford University MSDS
-79.70	PHYSPROP

dibutyl sulfone C8H18O2S[3, 64]

Compound Data

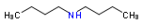


Melting point	**44.50 °C**	**317.65 K**			
CSID	62236	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	178.2923	**H bond donors**	0	**ACD/LogP**	2.00
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	0.98 g/cm^3
SMILES	O=S(=O)(CCCC)CCCC				
STD InChIKey	AIDFJGKWTOULTC-UHFFFAOYAR				

Melting Points

mp °C	source
44.00	Alfa Aesar
45.00	PHYSPROP

dibutylamine C8H19N[3, 31, 61, 64]



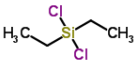
Compound Data

Melting point	**-61.50 °C**	**211.65 K**			
CSID	7856	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.2432	**H bond donors**	1	**ACD/LogP**	2.76
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.76 g/cm^3
SMILES	N(CCCC)CCCC				
STD InChIKey	JQVDAXLFBXTEQA-UHFFFAOYAO				

Melting Points

mp °C	source
-62.00	Alfa Aesar
-62.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-60.00	Oxford University MSDS
-62.00	PHYSPROP

dichlorodiethylsilane C4H10Cl2Si[3, 64]



Compound Data

Melting point	**-96.75 °C**	**176.40 K**			
CSID	14830	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	157.1137	**H bond donors**	0	**ACD/LogP**	4.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.03 g/cm^3
SMILES	Cl[Si](Cl)(CC)CC				
STD InChIKey	BYLOHCRAPOSXLY-UHFFFAOYAW				

Melting Points

mp °C	source
-97.00	Alfa Aesar
-96.50	PHYSPROP

dichloromethane CH2Cl2[3, 31, 61, 64]

Compound Data

Melting point	**-95.53 °C**	**177.62 K**			
CSID	6104	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.9326	**H bond donors**	0	**ACD/LogP**	1.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	ClCCl				
STD InChIKey	YMWUJEATGCHHMB-UHFFFAOYAG				

Melting Points

mp °C	source
-95.00	Alfa Aesar
-95.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-97.00	Oxford University MSDS
-95.10	PHYSPROP

dicofol C14H9Cl5O[61, 64]

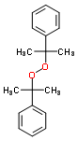
Compound Data

Melting point	**78.00 °C**	**351.15 K**			
CSID	7970	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	370.4857	**H bond donors**	1	**ACD/LogP**	5.74
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.53 g/cm^3
SMILES	Clc1ccc(cc1)C(O)(c2ccc(Cl)cc2)C(Cl)(Cl)Cl				
STD InChIKey	UOAMTSKGCBMZTC-UHFFFAOYAZ				

Melting Points

mp °C	source
78.50	Oxford University MSDS
77.50	PHYSPROP

dicumyl peroxide C18H22O2[61, 64]



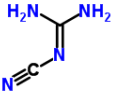
Compound Data

Melting point	**40.30 °C**	**313.45 K**			
CSID	6389	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	270.3661	**H bond donors**	0	**ACD/LogP**	5.71
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.03 g/cm^3
SMILES	O(OC(c1ccccc1)(C)C)C(c2ccccc2)(C)C				
STD InChIKey	XMNIXWIUMCBBBL-UHFFFAOYAA				

Melting Points

mp °C	source
40.00	Oxford University MSDS
40.60	PHYSPROP

dicyandiamide C2H4N4[3, 61, 64]



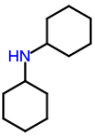
Compound Data

Melting point	**209.67 °C**	**482.82 K**			
CSID	9611	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	84.08	**H bond donors**	4	**ACD/LogP**	-1.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	N#C\N=C(/N)N				
STD InChIKey	QGBSISYHAICWAH-UHFFFAOYAY				

Melting Points

mp °C	source
210.00	Alfa Aesar
208.00	Oxford University MSDS
211.00	PHYSPROP

dicyclohexylamine C12H23N[2, 3, 61, 64]



Compound Data

Melting point	**-1.27 °C**	**271.88 K**			
CSID	7301	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	181.3177	**H bond donors**	1	**ACD/LogP**	3.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.91 g/cm^3
SMILES	N(C1CCCCC1)C2CCCCC2				
STD InChIKey	XBPCUCUWBYBCDP-UHFFFAOYAM				

Melting Points

mp °C	source
-2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-2.00	Alfa Aesar
-1.00	Oxford University MSDS
-0.10	PHYSPROP

diethoxymethane C5H12O2[3, 64]

Compound Data

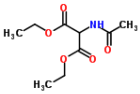
Melting point	**-66.25 °C**	**206.90 K**			
CSID	9630	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	104.1476	**H bond donors**	0	**ACD/LogP**	0.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.84 g/cm^3
SMILES	O(CC)COCC				
STD InChIKey	KLKFAASOGCDTDT-UHFFFAOYAH				

Melting Points

mp °C	source
-66.00	Alfa Aesar

-66.50	PHYSPROP

diethyl acetamidomalonate C9H15NO5[3, 64]



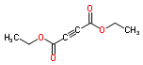
Compound Data

Melting point	**97.15 °C**	**370.30 K**			
CSID	13422	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	217.2191	**H bond donors**	1	**ACD/LogP**	0.36
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.14 g/cm^3
SMILES	O=C(NC(C(=O)OCC)C(=O)OCC)C				
STD InChIKey	ISOLMABRZPQKOV-UHFFFAOYAP				

Melting Points

mp °C	source
98.00	Alfa Aesar
96.30	PHYSPROP

diethyl acetylenedicarboxylate C8H10O4[3, 64]



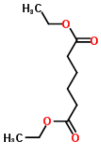
Compound Data

Melting point	**1.75 °C**	**274.90 K**			
CSID	63002	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	170.1626	**H bond donors**	0	**ACD/LogP**	2.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.13 g/cm^3
SMILES	CCOC(=O)C#CC(=O)OCC				
STD InChIKey	STRNXFOUBFLVIN-UHFFFAOYAZ				

Melting Points

mp °C	source
2.00	Alfa Aesar
1.50	PHYSPROP

diethyl adipate C10H18O4[2, 3, 64]



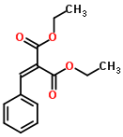
Compound Data

Melting point	**-19.27 °C**	**253.88 K**			
CSID	13835108	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	202.2475	**H bond donors**	0	**ACD/LogP**	2.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	1.01 g/cm^3
SMILES	CCOC(=O)CCCCC(=O)OCC				
STD InChIKey	VIZORQUEIQEFRT-UHFFFAOYAR				

Melting Points

mp °C	source
-18.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-20.00	Alfa Aesar
-19.80	PHYSPROP

diethyl benzylidenemalonate C14H16O4[3, 64]



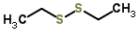
Compound Data

Melting point	**31.00 °C**	**304.15 K**			
CSID	85490	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	248.2744	**H bond donors**	0	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.13 g/cm^3
SMILES	O=C(OCC)C(/C(=O)OCC)=C\c1ccccc1				
STD InChIKey	VUWPIBNKJSEYIN-UHFFFAOYAT				

Melting Points

mp °C	source
30.00	Alfa Aesar
32.00	PHYSPROP

diethyl disulfide C4H10S2[3, 64]



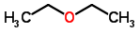
Compound Data

Melting point	**-101.75 °C**	**171.40 K**			
CSID	7786	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	122.2522	**H bond donors**	0	**ACD/LogP**	2.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.00 g/cm^3
SMILES	S(SCC)CC				
STD InChIKey	CETBSQOFQKLHHZ-UHFFFAOYAU				

Melting Points

mp °C	source
-102.00	Alfa Aesar
-101.50	PHYSPROP

diethyl ether C4H10O[3, 4, 61, 64]



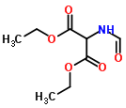
Compound Data

Melting point	**-116.08 °C**	**157.07 K**			
CSID	3168	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	74.1216	**H bond donors**	0	**ACD/LogP**	1.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.73 g/cm^3
SMILES	CCOCC				
STD InChIKey	RTZKZFJDLAIYFH-UHFFFAOYAB				

Melting Points

mp °C	source
-116.00	Alfa Aesar
-116.00	American Petroleum Institute. Research Project 44; Selected ...
-116.00	Oxford University MSDS
-116.30	PHYSPROP

diethyl formamidomalonate C8H13NO5[3, 64]



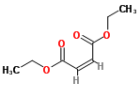
Compound Data

Melting point	**50.75 °C**	**323.90 K**			
CSID	72806	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	203.1925	**H bond donors**	1	**ACD/LogP**	1.05
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OCC)C(C(=O)OCC)NC=O				
STD InChIKey	PFLHGSJLYNJIOF-UHFFFAOYAQ				

Melting Points

mp °C	source
53.00	Alfa Aesar
48.50	PHYSPROP

diethyl maleate C8H12O4[2, 3, 61, 64]



Compound Data

Melting point	**-9.95 °C**	**263.20 K**			
CSID	4436353	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	172.1785	**H bond donors**	0	**ACD/LogP**	1.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	1.07 g/cm^3
SMILES	O=C(OCC)\C=C/C(=O)OCC				
STD InChIKey	IEPRKVQEAMIZSS-WAYWQWQTBX				

Melting Points

mp °C	source
-10.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-11.00	Alfa Aesar
-10.00	Oxford University MSDS

-8.80	PHYSPROP

diethyl maleate C8H18O5[3, 32, 61, 64]

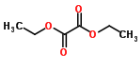
Compound Data

Melting point	**-5.60 °C**	**267.55 K**			
CSID	7908	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	194.2255	**H bond donors**	2	**ACD/LogP**	-2.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	12	**Predicted density**	1.11 g/cm^3
SMILES	OCCOCCOCCOCCO				
STD InChIKey	UWHCKJMYHZGTIT-UHFFFAOYAB				

Melting Points

mp °C	source
-4.00	Alfa Aesar
-6.20	DrugBank
-6.00	Oxford University MSDS
-6.20	PHYSPROP

diethyl oxalate C6H10O4[2, 3, 61, 64]



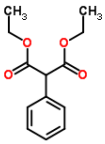
Compound Data

Melting point	**-40.65 °C**	**232.50 K**			
CSID	6998	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	146.1412	**H bond donors**	0	**ACD/LogP**	0.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.09 g/cm^3
SMILES	O=C(OCC)C(=O)OCC				
STD InChIKey	WYACBZDAHNBPPB-UHFFFAOYAA				

Melting Points

mp °C	source
-41.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-40.00	Alfa Aesar
-41.00	Oxford University MSDS
-40.60	PHYSPROP

diethyl phenylmalonate C13H16O4[2, 3, 64]



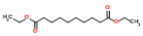
Compound Data

Melting point	**16.17 °C**	**289.32 K**			
CSID	59885	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	236.2637	**H bond donors**	0	**ACD/LogP**	2.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.11 g/cm^3
SMILES	O=C(OCC)C(C(=O)OCC)c1ccccc1				
STD InChIKey	FGYDHYCFHBSNPE-UHFFFAOYAH				

Melting Points

mp °C	source
16.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
16.00	Alfa Aesar
16.50	PHYSPROP

diethyl sebacate C14H26O4[2, 64]



Compound Data

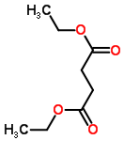
Melting point	**3.50 °C**	**276.65 K**			
CSID	7758	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	258.3538	**H bond donors**	0	**ACD/LogP**	3.85
Phase 25 °C	liquid/gas	**Rotatable bonds**	13	**Predicted density**	0.97 g/cm^3
SMILES	O=C(OCC)CCCCCCCCC(=O)OCC				
STD InChIKey	ONKUXPIBXRRIDU-UHFFFAOYAF				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
5.00	PHYSPROP

diethyl succinate C8H14O4[2, 3, 64]

Compound Data



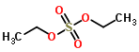
Melting point	**-20.67 °C**	**252.48 K**			
CSID	13865630	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1944	**H bond donors**	0	**ACD/LogP**	1.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.04 g/cm^3
SMILES	O=C(CCC(=O)OCC)OCC				
STD InChIKey	DKMROQRQHGEIOW-UHFFFAOYAX				

Melting Points

mp °C	source
-20.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-21.00	Alfa Aesar
-21.00	PHYSPROP

diethyl sulfate C4H10O4S[3, 61, 64]

Compound Data



Melting point	**-24.33 °C**	**248.82 K**			
CSID	5931	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	154.1848	**H bond donors**	0	**ACD/LogP**	1.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	O=S(=O)(OCC)OCC				
STD InChIKey	DENRZWYUOJLTMF-UHFFFAOYAR				

Melting Points

mp °C	source
-25.00	Alfa Aesar
-24.00	Oxford University MSDS
-24.00	PHYSPROP

diethyl sulfide C4H10S[3, 4, 64]

Compound Data

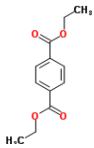
Melting point	**-103.97 °C**	**169.18 K**			
CSID	9233	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	90.1872	**H bond donors**	0	**ACD/LogP**	1.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.83 g/cm^3
SMILES	S(CC)CC				
STD InChIKey	LJSQFQKUNVCTIA-UHFFFAOYAZ				

Melting Points

mp °C	source
-104.00	Alfa Aesar
-104.00	American Petroleum Institute. Research Project 44; Selected ...
-103.90	PHYSPROP

diethyl terephthalate C12H14O4[3, 64]

Compound Data



Melting point	**44.50 °C**	**317.65 K**			
CSID	11972	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	222.2372	**H bond donors**	0	**ACD/LogP**	3.54
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.12 g/cm^3
SMILES	O=C(OCC)c1ccc(C(=O)OCC)cc1				

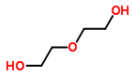
STD InChIKey	ONIHPYYWNBVMID-UHFFFAOYAS

Melting Points

mp °C	source
45.00	Alfa Aesar
44.00	PHYSPROP

diethylene glycol C4H10O3[3, 64]

Compound Data



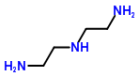
Melting point	**-10.20 °C**	**262.95 K**			
CSID	13835180	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	106.1204	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	1.11 g/cm^3
SMILES	C(COCCO)O				
STD InChIKey	MTHSVFCYNBDYFN-UHFFFAOYAK				

Melting Points

mp °C	source
-10.00	Alfa Aesar
-10.40	PHYSPROP

diethylenetriamine C4H13N3[3, 61, 64]

Compound Data



Melting point	**-38.00 °C**	**235.15 K**			
CSID	13835401	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	103.1661	**H bond donors**	5	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.93 g/cm^3
SMILES	C(CNCCN)N				
STD InChIKey	RPNUMPOLZDHAAY-UHFFFAOYAH				

Melting Points

mp °C	source
-40.00	Alfa Aesar
-35.00	Oxford University MSDS
-39.00	PHYSPROP

diethylsilane C4H12Si[3, 64]

Compound Data

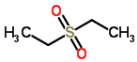
Melting point	**-133.15 °C**	**140.00 K**			
CSID	61632	**H bond acceptors**	0	**Rule of 5 violations**	NA
Molecular weight	88.2236	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.00 g/cm^3
SMILES	CC[SiH2]CC				
STD InChIKey	UCXUKTLCVSGCNR-UHFFFAOYAD				

Melting Points

mp °C	source
-132.00	Alfa Aesar
-134.30	PHYSPROP

diethylsulfone C4H10O2S[3, 64]

Compound Data



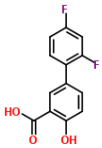
Melting point	**72.75 °C**	**345.90 K**			
CSID	62226	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.186	**H bond donors**	0	**ACD/LogP**	-0.13
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	O=S(=O)(CC)CC				
STD InChIKey	MBDUIEKYVPVZJH-UHFFFAOYAH				

Melting Points

mp °C	source
72.00	Alfa Aesar
73.50	PHYSPROP

diflunisal C13H8F2O3[32, 35, 44, 56, 64]

Compound Data



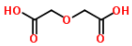
Melting point	**213.50 °C**	**486.65 K**			
CSID	2951	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	250.1976	**H bond donors**	2	**ACD/LogP**	4.44
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.44 g/cm^3
SMILES	O=C(O)c1cc(ccc1O)c2ccc(F)cc2F				
STD InChIKey	HUPFGZXOMWLGNK-UHFFFAOYAE				

Melting Points

mp °C	source
215.50	DrugBank
215.50	EPISuite-ChemSpider
210.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
210.50	Merck Index
215.50	PHYSPROP

diglycolic acid C4H6O5[3, 64]

Compound Data



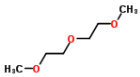
Melting point	**145.50 °C**	**418.65 K**			
CSID	7797	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	134.0874	**H bond donors**	2	**ACD/LogP**	-2.09
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.49 g/cm^3
SMILES	O=C(O)COCC(=O)O				
STD InChIKey	QEVGZEDELICMKH-UHFFFAOYAA				

Melting Points

mp °C	source
143.00	Alfa Aesar
148.00	PHYSPROP

diglyme C6H14O3[2, 3, 64]

Compound Data



Melting point	**-65.33 °C**	**207.82 K**			
CSID	13839575	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	134.1736	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.91 g/cm^3
SMILES	COCCOCCOC				
STD InChIKey	SBZXBUIDTXKZTM-UHFFFAOYAG				

Melting Points

mp °C	source
-64.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-64.00	Alfa Aesar
-68.00	PHYSPROP

dihydrobenzofuran C8H8O[3, 64]

Compound Data

Melting point	**-21.25 °C**	**251.90 K**			
CSID	21106522	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	120.1485	**H bond donors**	0	**ACD/LogP**	2.14
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.10 g/cm^3

SMILES	c1cccc2OCCc12
STD InChIKey	HBEDSQVIWPRPAY-UHFFFAOYAI

Melting Points

mp °C	source
-21.00	Alfa Aesar
-21.50	PHYSPROP

diiodomethane CH2I2[3, 31, 61, 64]

Compound Data

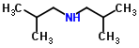
Melting point	**5.78 °C**	**278.92 K**			
CSID	6106	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	267.8355	**H bond donors**	0	**ACD/LogP**	2.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	3.24 g/cm^3
SMILES	ICI				
STD InChIKey	NZZFYRREKKOMAT-UHFFFAOYAO				

Melting Points

mp °C	source
6.00	Alfa Aesar
6.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
5.00	Oxford University MSDS
6.10	PHYSPROP

diisobutylamine C8H19N[3, 64]

Compound Data



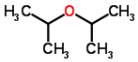
Melting point	**-75.25 °C**	**197.90 K**			
CSID	7794	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.2432	**H bond donors**	1	**ACD/LogP**	2.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.76 g/cm^3
SMILES	N(CC(C)C)CC(C)C				
STD InChIKey	NJBCRXCAPCODGX-UHFFFAOYAJ				

Melting Points

mp °C	source
-77.00	Alfa Aesar
-73.50	PHYSPROP

diisopropyl ether C6H14O[4, 64]

Compound Data



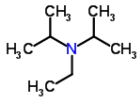
Melting point	**-86.40 °C**	**186.75 K**			
CSID	7626	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	102.1748	**H bond donors**	0	**ACD/LogP**	1.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.76 g/cm^3
SMILES	O(C(C)C)C(C)C				
STD InChIKey	ZAFNJMIOTHYJRJ-UHFFFAOYAC				

Melting Points

mp °C	source
-86.00	American Petroleum Institute. Research Project 44; Selected ...
-86.80	PHYSPROP

diisopropylethylamine C8H19N[3, 61]

Compound Data



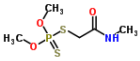
Melting point	**-48.00 °C**	**225.15 K**			
CSID	73565	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.2432	**H bond donors**	0	**ACD/LogP**	2.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.77 g/cm^3
SMILES	N(C(C)C)(C(C)C)CC				
STD InChIKey	JGFZNNIVVJXRND-UHFFFAOYAV				

Melting Points

mp °C	source
-46.00	Alfa Aesar
-50.00	Oxford University MSDS

dimethoate C5H12NO3PS2[61, 64]

Compound Data



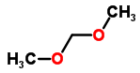
Melting point	**51.75 °C**	**324.90 K**			
CSID	2973	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	229.2574	**H bond donors**	1	**ACD/LogP**	0.48
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.30 g/cm^3
SMILES	O=C(NC)CSP(=S)(OC)OC				
STD InChIKey	MCWXGJITAZMZEV-UHFFFAOYAB				

Melting Points

mp °C	source
51.50	Oxford University MSDS
52.00	PHYSPROP

dimethoxymethane C3H8O2[2, 3, 61, 64]

Compound Data



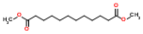
Melting point	**-104.95 °C**	**168.20 K**			
CSID	13837190	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	76.0944	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.84 g/cm^3
SMILES	COCOC				
STD InChIKey	NKDDWNXOKDWJAK-UHFFFAOYAE				

Melting Points

mp °C	source
-105.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-105.00	Alfa Aesar
-105.00	Oxford University MSDS
-104.80	PHYSPROP

dimethyl 1,10-decanedicarboxylate C14H26O4[3, 64]

Compound Data



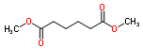
Melting point	**30.95 °C**	**304.10 K**			
CSID	67007	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	258.3538	**H bond donors**	0	**ACD/LogP**	3.85
Phase 25 °C	solid	**Rotatable bonds**	13	**Predicted density**	0.97 g/cm^3
SMILES	O=C(OC)CCCCCCCCCCC(=O)OC				
STD InChIKey	IZMOTZDBVPMOFE-UHFFFAOYAP				

Melting Points

mp °C	source
30.00	Alfa Aesar
31.90	PHYSPROP

dimethyl adipate C8H14O4[2, 3, 61, 64]

Compound Data



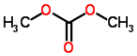
Melting point	**8.57 °C**	**281.72 K**			
CSID	11824	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1944	**H bond donors**	0	**ACD/LogP**	1.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.04 g/cm^3
SMILES	O=C(OC)CCCCC(=O)OC				
STD InChIKey	UDSFAEKRVUSQDD-UHFFFAOYAJ				

Melting Points

mp °C	source
8.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
8.00	Alfa Aesar
8.00	Oxford University MSDS
10.30	PHYSPROP

dimethyl carbonate C3H6O3[2, 3, 61, 64]

Compound Data



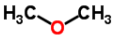
Melting point	**2.75 °C**	**275.90 K**			
CSID	11526	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	90.0779	**H bond donors**	0	**ACD/LogP**	0.07
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.02 g/cm^3
SMILES	COC(=O)OC				
STD InChIKey	IEJIGPNLZYLLBP-UHFFFAOYAC				

Melting Points

mp °C	source
3.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
4.00	Alfa Aesar
1.00	Oxford University MSDS
3.00	PHYSPROP

dimethyl ether C2H6O[61, 64]

Compound Data



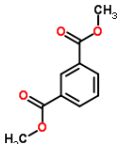
Melting point	**-139.75 °C**	**133.40 K**			
CSID	7956	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	46.0684	**H bond donors**	0	**ACD/LogP**	0.02
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.68 g/cm^3
SMILES	COC				
STD InChIKey	LCGLNKUTAGEVQW-UHFFFAOYAU				

Melting Points

mp °C	source
-138.00	Oxford University MSDS
-141.50	PHYSPROP

dimethyl isophthalate C10H10O4[3, 64]

Compound Data

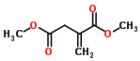


Melting point	**68.25 °C**	**341.40 K**			
CSID	14360	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	2.45
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(OC)c1cccc(C(=O)OC)c1				
STD InChIKey	VNGOYPQMJFJDLV-UHFFFAOYAW				

Melting Points

mp °C	source
69.00	Alfa Aesar
67.50	PHYSPROP

dimethyl itaconate C7H10O4[3, 64]



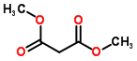
Compound Data

Melting point	**37.00 °C**	**310.15 K**			
CSID	62453	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	158.1519	**H bond donors**	0	**ACD/LogP**	0.62
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.08 g/cm^3
SMILES	COC(=O)CC(=C)C(=O)OC				
STD InChIKey	ZWWQRMFIZFPUAA-UHFFFAOYAN				

Melting Points

mp °C	source
36.00	Alfa Aesar
38.00	PHYSPROP

dimethyl malonate C5H8O4[2, 3, 61, 64]



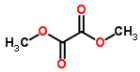
Compound Data

Melting point	**-61.98 °C**	**211.17 K**			
CSID	21106102	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	132.1146	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.12 g/cm^3
SMILES	COC(=O)CC(=O)OC				
STD InChIKey	BEPAFCGSDWSTEL-UHFFFAOYAJ				

Melting Points

mp °C	source
-62.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-62.00	Alfa Aesar
-62.00	Oxford University MSDS
-61.90	PHYSPROP

dimethyl oxalate C4H6O4[2, 3, 61, 64]



Compound Data

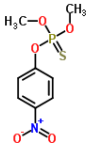
Melting point	**52.77 °C**	**325.92 K**			
CSID	10649	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	118.088	**H bond donors**	0	**ACD/LogP**	-0.34
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	O=C(OC)C(=O)OC				
STD InChIKey	LOMVENUNSWAXEN-UHFFFAOYAF				

Melting Points

mp °C	source
52.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
52.00	Alfa Aesar
54.30	PHYSPROP
	Values not used in calculating the average melting point
-54.00	Oxford University MSDS[1]

1. inverted sign JCB

dimethyl parathion C8H10NO5PS[61, 64]



Compound Data

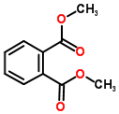
Melting point	**35.75 °C**	**308.90 K**			
CSID	3987	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	263.2075	**H bond donors**	0	**ACD/LogP**	2.78
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.41 g/cm^3
SMILES	S=P(Oc1ccc(cc1)[N+]([O-])=O)(OC)OC				
STD InChIKey	RLBIQVVOMOPOHC-UHFFFAOYAW				

Melting Points

mp °C	source
36.00	Oxford University MSDS

35.50	PHYSPROP

dimethyl phthalate C10H10O4[2, 3, 61, 64]



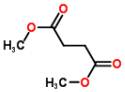
Compound Data

Melting point	**3.62 °C**	**276.77 K**			
CSID	13837329	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	1.64
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(OC)c1ccccc1C(=O)OC				
STD InChIKey	NIQCNGHVCWTJSM-UHFFFAOYAF				

Melting Points

mp °C	source
2.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
5.00	Alfa Aesar
2.00	Oxford University MSDS
5.50	PHYSPROP

dimethyl succinate C6H10O4[2, 3, 61, 64]



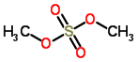
Compound Data

Melting point	**19.12 °C**	**292.27 K**			
CSID	13848341	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	146.1412	**H bond donors**	0	**ACD/LogP**	0.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.09 g/cm^3
SMILES	O=C(OC)CCC(=O)OC				
STD InChIKey	MUXOBHXGJLMRAB-UHFFFAOYAP				

Melting Points

mp °C	source
19.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
19.00	Alfa Aesar
19.50	Oxford University MSDS
19.00	PHYSPROP

dimethyl sulfate C2H6O4S[61, 64]



Compound Data

Melting point	**-29.50 °C**	**243.65 K**			
CSID	6252	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	126.1316	**H bond donors**	0	**ACD/LogP**	0.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	COS(=O)(=O)OC				
STD InChIKey	VAYGXNSJCAHWJZ-UHFFFAOYAK				

Melting Points

mp °C	source
-32.00	Oxford University MSDS
-27.00	PHYSPROP

dimethyl sulfone C2H6O2S[3, 61, 64]

Compound Data

Melting point	**109.33 °C**	**382.48 K**			
CSID	5978	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	94.1328	**H bond donors**	0	**ACD/LogP**	-1.19
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	O=S(=O)(C)C				
STD InChIKey	HHVIBTZHLRERCL-UHFFFAOYAG				

Melting Points

mp °C	source
110.00	Alfa Aesar
109.00	Oxford University MSDS
109.00	PHYSPROP

dimethyl sulfoxide C2H6OS[2, 3, 32, 61, 64]

Compound Data

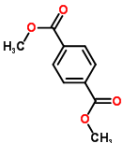
Melting point	**18.28 °C**	**291.43 K**			
CSID	659	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	78.1334	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.10 g/cm^3
SMILES	CS(=O)C				
STD InChIKey	IAZDPXIOMUYVGZ-UHFFFAOYAR				

Melting Points

mp °C	source
18.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
18.00	Alfa Aesar
18.50	DrugBank
18.40	Oxford University MSDS
18.50	PHYSPROP

dimethyl terephthalate C10H10O4[2, 3, 61, 64]

Compound Data



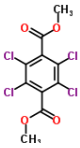
Melting point	**141.25 °C**	**414.40 K**			
CSID	13863300	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	2.47
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(OC)c1ccc(cc1)C(=O)OC				
STD InChIKey	WOZVHXUHUFLZGK-UHFFFAOYAP				

Melting Points

mp °C	source
141.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
142.00	Alfa Aesar
141.00	Oxford University MSDS
141.00	PHYSPROP

dimethyl tetrachloroterephthalate C10H6Cl4O4[3, 64]

Compound Data



Melting point	**156.00 °C**	**429.15 K**			
CSID	2839	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	331.9642	**H bond donors**	0	**ACD/LogP**	3.48
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.56 g/cm^3
SMILES	Clc1c(C(=O)OC)c(Cl)c(Cl)c(C(=O)OC)c1Cl				
STD InChIKey	NPOJQCVWMSKXDN-UHFFFAOYAS				

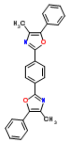
Melting Points

mp °C	source
157.00	Alfa Aesar
155.00	PHYSPROP

dimethyl-POPOP C26H20N2O2[3, 61]

Compound Data

Melting point	**233.00 °C**	**506.15 K**			
CSID	68961	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	392.4492	**H bond donors**	0	**ACD/LogP**	7.37
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	3



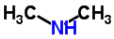
					1.17 g/cm
SMILES	n1c(c(oc1c4ccc(c2nc(c(o2)c3ccccc3)C)cc4)c5ccccc5)C				
STD InChIKey	VLDFXDUAENINOO-UHFFFAOYAN				

Melting Points

mp °C	source
234.00	Alfa Aesar
232.00	Oxford University MSDS

dimethylamine C2H7N[31, 61, 64]

Compound Data



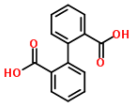
Melting point	**-92.07 °C**	**181.08 K**			
CSID	654	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	45.0837	**H bond donors**	1	**ACD/LogP**	-0.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.64 g/cm^3
SMILES	N(C)C				
STD InChIKey	ROSDSFDQCJNGOL-UHFFFAOYAM				

Melting Points

mp °C	source
-92.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-92.00	Oxford University MSDS
-92.20	PHYSPROP

diphenic acid C14H10O4[3, 64]

Compound Data



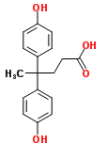
Melting point	**231.25 °C**	**504.40 K**			
CSID	9795	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	242.2268	**H bond donors**	2	**ACD/LogP**	1.74
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.35 g/cm^3
SMILES	c1ccc(c(c1)c2ccccc2C(=O)O)C(=O)O				
STD InChIKey	GWZCCUDJHOGOSO-UHFFFAOYAZ				

Melting Points

mp °C	source
229.00	Alfa Aesar
233.50	PHYSPROP

diphenolic acid C17H18O4[3, 64]

Compound Data



Melting point	**172.25 °C**	**445.40 K**			
CSID	60518	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	286.3224	**H bond donors**	3	**ACD/LogP**	2.89
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.26 g/cm^3
SMILES	O=C(O)CCC(c1ccc(O)cc1)(c2ccc(O)cc2)C				
STD InChIKey	VKOUCJUTMGHNOR-UHFFFAOYAX				

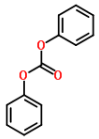
Melting Points

mp °C	source
173.00	Alfa Aesar
171.50	PHYSPROP

diphenyl carbonate C13H10O3[3, 61, 64]

Compound Data

Melting point	**80.33 °C**	**353.48 K**	



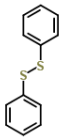
CSID	7315	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.2167	**H bond donors**	0	**ACD/LogP**	3.28
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.20 g/cm^3
SMILES	O=C(Oc1ccccc1)Oc2ccccc2				
STD InChIKey	ROORDVPLFPIABK-UHFFFAOYAY				

Melting Points

mp °C	source
79.00	Alfa Aesar
79.00	Oxford University MSDS
83.00	PHYSPROP

diphenyl disulfide C12H10S2[3, 64]

Compound Data



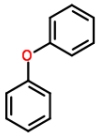
Melting point	**61.00 °C**	**334.15 K**			
CSID	12861	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	218.3378	**H bond donors**	0	**ACD/LogP**	4.41
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	c1ccc(cc1)SSc2ccccc2				
STD InChIKey	GUUVPOWQJOLRAS-UHFFFAOYAY				

Melting Points

mp °C	source
60.00	Alfa Aesar
62.00	PHYSPROP

diphenyl ether C12H10O[2, 3, 61, 64]

Compound Data



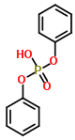
Melting point	**27.45 °C**	**300.60 K**			
CSID	7302	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2072	**H bond donors**	0	**ACD/LogP**	4.21
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.06 g/cm^3
SMILES	O(c1ccccc1)c2ccccc2				
STD InChIKey	USIUVYZYUHIAEV-UHFFFAOYAV				

Melting Points

mp °C	source
28.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
28.00	Alfa Aesar
27.00	Oxford University MSDS
26.80	PHYSPROP

diphenyl phosphoric acid C12H11O4P[3, 64]

Compound Data

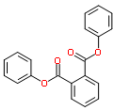


Melting point	**66.75 °C**	**339.90 K**			
CSID	12722	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	250.1871	**H bond donors**	1	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.34 g/cm^3
SMILES	O=P(Oc1ccccc1)(Oc2ccccc2)O				
STD InChIKey	ASMQGLCHMVWBQR-UHFFFAOYAM				

Melting Points

mp °C	source
66.00	Alfa Aesar
67.50	PHYSPROP

diphenyl phthalate C20H14O4[3, 64]



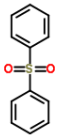
Compound Data

Melting point	**74.00 °C**	**347.15 K**			
CSID	6520	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	318.3228	**H bond donors**	0	**ACD/LogP**	4.41
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.24 g/cm^3
SMILES	O=C(Oc1ccccc1)c3ccccc3C(=O)Oc2ccccc2				
STD InChIKey	DWNAQMUDCDVSLT-UHFFFAOYAG				

Melting Points

mp °C	source
75.00	Alfa Aesar
73.00	PHYSPROP

diphenyl sulfone C12H10O2S[3, 64]



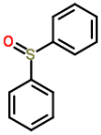
Compound Data

Melting point	**128.25 °C**	**401.40 K**			
CSID	29117	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	218.2716	**H bond donors**	0	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=S(=O)(c1ccccc1)c2ccccc2				
STD InChIKey	KZTYYGOKRVBIMI-UHFFFAOYAU				

Melting Points

mp °C	source
128.00	Alfa Aesar
128.50	PHYSPROP

diphenyl sulfoxide C12H10OS[2, 3, 64]



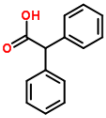
Compound Data

Melting point	**70.73 °C**	**343.88 K**			
CSID	13090	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	202.2722	**H bond donors**	0	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	O=S(c1ccccc1)c2ccccc2				
STD InChIKey	JJHHIJFTHRNPIK-UHFFFAOYAI				

Melting Points

mp °C	source
70.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
71.00	Alfa Aesar
71.20	PHYSPROP

diphenylacetic acid C14H12O2[3, 35, 48, 64]



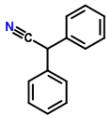
Compound Data

Melting point	**146.75 °C**	**419.90 K**			
CSID	8030	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.2439	**H bond donors**	1	**ACD/LogP**	3.25
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)C(c1ccccc1)c2ccccc2				
STD InChIKey	PYHXGXCGESYPCW-UHFFFAOYAC				

Melting Points

mp °C	source
147.00	Alfa Aesar
147.00	EPISuite-ChemSpider
146.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
147.00	PHYSPROP

diphenylacetonitrile C14H11N[3, 64]



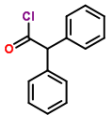
Compound Data

Melting point	**74.15 °C**	**347.30 K**			
CSID	6576	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	193.2438	**H bond donors**	0	**ACD/LogP**	3.30
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.08 g/cm^3
SMILES	N#CC(c1ccccc1)c2ccccc2				
STD InChIKey	NEBPTMCRLHKPOB-UHFFFAOYAI				

Melting Points

mp °C	source
74.00	Alfa Aesar
74.30	PHYSPROP

diphenylacetyl chloride C14H11ClO[3, 64]



Compound Data

Melting point	**54.75 °C**	**327.90 K**			
CSID	67212	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	230.6895	**H bond donors**	0	**ACD/LogP**	3.96
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.19 g/cm^3
SMILES	O=C(Cl)C(c1ccccc1)c2ccccc2				
STD InChIKey	MSYLETHDEIJMAF-UHFFFAOYAP				

Melting Points

mp °C	source
53.00	Alfa Aesar
56.50	PHYSPROP

diphenylacetylene C14H10[2, 3, 48, 61, 64]

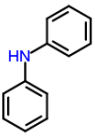
Compound Data

Melting point	**61.10 °C**	**334.25 K**			
CSID	9961	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	178.2292	**H bond donors**	0	**ACD/LogP**	4.73
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	c1ccc(cc1)C#Cc2ccccc2				
STD InChIKey	JRXXLCKWQFKACW-UHFFFAOYAN				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
60.00	Alfa Aesar
63.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
60.00	Oxford University MSDS
62.50	PHYSPROP

diphenylamine C12H11N[3, 61, 64, 70]



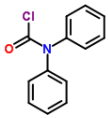
Compound Data

Melting point	**52.98 °C**	**326.12 K**			
CSID	11003	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	169.2224	**H bond donors**	1	**ACD/LogP**	3.36
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.09 g/cm^3
SMILES	c1ccc(cc1)Nc2ccccc2				
STD InChIKey	DMBHHRLKUKUOEG-UHFFFAOYAJ				

Melting Points

mp °C	source
54.00	Alfa Aesar
53.00	Oxford University MSDS
52.90	PHYSPROP
52.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

diphenylcarbamyl chloride C13H10ClNO[3, 64]



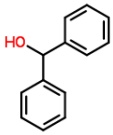
Compound Data

Melting point	**83.50 °C**	**356.65 K**			
CSID	59164	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	231.6776	**H bond donors**	0	**ACD/LogP**	3.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	O=C(Cl)N(c1ccccc1)c2ccccc2				
STD InChIKey	XNBKKRFABABBPM-UHFFFAOYAY				

Melting Points

mp °C	source
84.00	Alfa Aesar
83.00	PHYSPROP

diphenylmethanol C13H12O[2, 3, 61, 64]



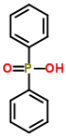
Compound Data

Melting point	**66.75 °C**	**339.90 K**			
CSID	6770	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.2338	**H bond donors**	1	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	OC(c1ccccc1)c2ccccc2				
STD InChIKey	QILSFLSDHQAZET-UHFFFAOYAG				

Melting Points

mp °C	source
66.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
66.00	Alfa Aesar
66.00	Oxford University MSDS
69.00	PHYSPROP

diphenylphosphinic acid C12H11O2P[3, 64]



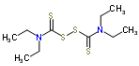
Compound Data

Melting point	**194.50 °C**	**467.65 K**			
CSID	14810	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	218.1883	**H bond donors**	1	**ACD/LogP**	1.61
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	O=P(O)(c1ccccc1)c2ccccc2				
STD InChIKey	BEQVQKJCLJBTKZ-UHFFFAOYAV				

Melting Points

mp °C	source
195.00	Alfa Aesar
194.00	PHYSPROP

disulfiram C10H20N2S4[3, 44, 61, 64]



Compound Data

Melting point	**70.62 °C**	**343.77 K**			
CSID	3005	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	296.5392	**H bond donors**	0	**ACD/LogP**	3.82
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.21 g/cm^3
SMILES	CCN(CC)C(=S)SSC(=S)N(CC)CC				
STD InChIKey	AUZONCFQVSMFAP-UHFFFAOYAF				

Melting Points

mp °C	source
71.00	Alfa Aesar
70.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...

70.00	Oxford University MSDS
71.50	PHYSPROP

dithiocyanomethane C3H2N2S2[3, 61]

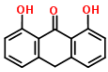
Compound Data

Melting point	**105.50 °C**	**378.65 K**			
CSID	21349	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1914	**H bond donors**	0	**ACD/LogP**	0.80
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.40 g/cm^3
SMILES	N#CSCSC#N				
STD InChIKey	JWZXKXIUSSIAMR-UHFFFAOYAO				

Melting Points

mp °C	source
105.00	Alfa Aesar
106.00	Oxford University MSDS

dithranol C14H10O3[3, 61, 64]



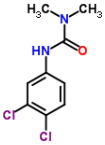
Compound Data

Melting point	**179.67 °C**	**452.82 K**			
CSID	2117	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	226.2274	**H bond donors**	2	**ACD/LogP**	4.16
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.42 g/cm^3
SMILES	O=C2c1c(O)cccc1Cc3c2c(O)ccc3				
STD InChIKey	NUZWLKWWNNJHPT-UHFFFAOYAS				

Melting Points

mp °C	source
179.00	Alfa Aesar
181.00	Oxford University MSDS
179.00	PHYSPROP

diuron C9H10Cl2N2O[3, 44, 64, 70]



Compound Data

Melting point	**158.38 °C**	**431.52 K**			
CSID	3008	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	233.0945	**H bond donors**	1	**ACD/LogP**	2.78
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.37 g/cm^3
SMILES	Clc1ccc(NC(=O)N(C)C)cc1Cl				
STD InChIKey	XMTQQYYKAHVGBJ-UHFFFAOYAZ				

Melting Points

mp °C	source
158.00	Alfa Aesar
158.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
158.00	PHYSPROP
159.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

docosane C22H46[3, 61, 64]

Compound Data

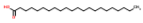
Melting point	**43.80 °C**	**316.95 K**			
CSID	11899	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	310.6006	**H bond donors**	0	**ACD/LogP**	12.45
Phase 25 °C	solid	**Rotatable bonds**	19	**Predicted density**	0.79 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCC)CCC				
STD InChIKey	HOWGUJZVBDQJKV-UHFFFAOYAZ				

Melting Points

mp °C	source
45.00	Alfa Aesar
42.00	Oxford University MSDS
44.40	PHYSPROP

docosanoic acid C22H44O2[3, 61, 64]

Compound Data



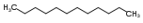
Melting point	**77.67 °C**	**350.82 K**			
CSID	7923	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	340.5836	**H bond donors**	1	**ACD/LogP**	10.34
Phase 25 °C	solid	**Rotatable bonds**	20	**Predicted density**	0.88 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCCCCCCCCC				
STD InChIKey	UKMSUNONTOPOIO-UHFFFAOYAN				

Melting Points

mp °C	source
76.00	Alfa Aesar
76.00	Oxford University MSDS
81.00	PHYSPROP

dodecane C12H26[3, 4, 32, 61, 64]

Compound Data



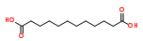
Melting point	**-9.76 °C**	**263.39 K**			
CSID	7890	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	170.3348	**H bond donors**	0	**ACD/LogP**	7.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.75 g/cm^3
SMILES	C(CCCCCCCC)CCC				
STD InChIKey	SNRUBQQJIBEYMU-UHFFFAOYAS				

Melting Points

mp °C	source
-10.00	Alfa Aesar
-10.00	American Petroleum Institute. Research Project 44; Selected ...
-9.60	DrugBank
-9.60	Oxford University MSDS
-9.60	PHYSPROP

dodecanedioic acid C12H22O4[3, 61, 64]

Compound Data



Melting point	**128.67 °C**	**401.82 K**			
CSID	12213	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	230.3007	**H bond donors**	2	**ACD/LogP**	2.92
Phase 25 °C	solid	**Rotatable bonds**	11	**Predicted density**	1.07 g/cm^3
SMILES	O=C(O)CCCCCCCCCCC(=O)O				
STD InChIKey	TVIDDXQYHWJXFK-UHFFFAOYAC				

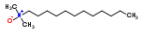
Melting Points

mp °C	source
129.00	Alfa Aesar
129.00	Oxford University MSDS
128.00	PHYSPROP

dodecyl dimethylamine N-oxide C14H31NO[61, 64]

Compound Data

Melting point	**131.50 °C**	**404.65 K**			
CSID	14688	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	229.402	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	solid	**Rotatable bonds**	11	**Predicted density**	[3]



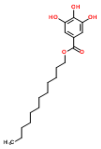
0.00 g/cm

SMILES	[O-][N+](CCCCCCCCCCCCC)(C)C
STD InChIKey	SYELZBGXAIXKHU-UHFFFAOYAJ

Melting Points

mp °C	source
132.50	Oxford University MSDS
130.50	PHYSPROP

dodecyl gallate C19H30O5[3, 64]



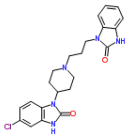
Compound Data

Melting point	**96.75 °C**	**369.90 K**			
CSID	13777	**H bond acceptors**	5	**Rule of 5 violations**	1
Molecular weight	338.4385	**H bond donors**	3	**ACD/LogP**	7.38
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	1.11 g/cm^3
SMILES	O=C(OCCCCCCCCCCCCC)c1cc(O)c(O)c(O)c1				
STD InChIKey	RPWFJAMTCNSJKK-UHFFFAOYAC				

Melting Points

mp °C	source
97.00	Alfa Aesar
96.50	PHYSPROP

domperidone C22H24ClN5O2[32, 61, 64]



Compound Data

Melting point	**240.83 °C**	**513.98 K**			
CSID	3039	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	425.9113	**H bond donors**	2	**ACD/LogP**	4.50
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.34 g/cm^3
SMILES	Clc1cc2c(cc1)N(C(=O)N2)C5CCN(CCCN4c3ccccc3NC4=O)CC5				
STD InChIKey	FGXWKSZFVQUSTL-UHFFFAOYAW				

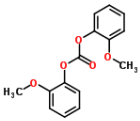
Melting Points

mp °C	source
242.50	DrugBank
237.50	Oxford University MSDS
242.50	PHYSPROP

dotriacontane C32H66[3, 64]

Compound Data

Melting point	**69.85 °C**	**343.00 K**			
CSID	10542	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	450.8664	**H bond donors**	0	**ACD/LogP**	17.76
Phase 25 °C	solid	**Rotatable bonds**	29	**Predicted density**	0.81 g/cm^3
SMILES	C(CCCCCCCCCCCCC



CSID	10633	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	274.2687	**H bond donors**	0	**ACD/LogP**	2.41
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.21 g/cm^3
SMILES	O=C(Oc1ccccc1OC)Oc2ccccc2OC				
STD InChIKey	ORUJFMPWKPVXLZ-UHFFFAOYAQ				

Melting Points

mp °C	source
87.00	Alfa Aesar
89.00	PHYSPROP

epichlorohydrin C3H5ClO[3, 61, 64, 64, 78]

Compound Data

Melting point	**-57.10 °C**	**216.05 K**			
CSID	13837112	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	92.5242	**H bond donors**	0	**ACD/LogP**	0.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	ClCC1CO1				
STD InChIKey	BRLQWZUYTZBJKN-UHFFFAOYAY				

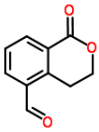
Melting Points

mp °C	source
-57.00	Alfa Aesar
-57.20	PHYSPROP
-57.10	WDTrade
	Values not used in calculating the average melting point
-26.00	Oxford University MSDS[1]
-26.00	PHYSPROP[2]

1. unlikely to be higher mp than bromo analog at -40C JCB
2. unlikely to be higher mp than bromo analog at -40C JCB

erythrocentaurin C10H8O3[9, 48, 64]

Compound Data



Melting point	**140.17 °C**	**413.32 K**			
CSID	165975	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	176.1687	**H bond donors**	0	**ACD/LogP**	0.75
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	O=Cc1cccc2C(=O)OCCc12				
STD InChIKey	TUADBWMDDLWUME-UHFFFAOYAR				

Melting Points

mp °C	source
140.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
140.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
140.50	PHYSPROP

ethane C2H6[14, 25, 40, 61, 64, 73, 83]

Compound Data

Melting point	**-183.01 °C**	**90.14 K**			
CSID	6084	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	30.069	**H bond donors**	0	**ACD/LogP**	1.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.49 g/cm^3
SMILES	CC				
STD InChIKey	OTMSDBZUPAUEDD-UHFFFAOYAK				

Melting Points

mp °C	source
-183.33	Burnett LJ; Muller BH. Journal of Chemical and Engineering D...

-182.85	Cheric
-182.78	Givens FL; McCormick WD. Journal of Chemical Physics 67(3) 1...
-182.79	PHYSPROP
-183.28	Witt RK; Kemp JD. Journal of the American Chemical Society 5...
	Values not used in calculating the average melting point
-172.00	Oxford University MSDS[1]
-172.15	Streng AG Journal of Chemical and Engineering Data 16(3) 357...[2]

1. clearly out of range JCB
2. clearly out of range JCB

ethanethiol C2H6S[3, 61, 64]

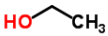
Compound Data

Melting point	**-147.93 °C**	**125.22 K**			
CSID	6103	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	62.134	**H bond donors**	0	**ACD/LogP**	1.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.82 g/cm^3
SMILES	CCS				
STD InChIKey	DNJIEGIFACGWOD-UHFFFAOYAW				

Melting Points

mp °C	source
-148.00	Alfa Aesar
-148.00	Oxford University MSDS
-147.80	PHYSPROP

ethanol C2H6O[4, 28, 32, 56, 61, 61, 64, 72, 81]



Compound Data

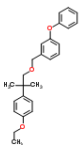
Melting point	**-114.13 °C**	**159.02 K**			
CSID	682	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	46.0684	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.78 g/cm^3
SMILES	CCO				
STD InChIKey	LFQSCWFLJHTTHZ-UHFFFAOYAB				

Melting Points

mp °C	source
-114.00	American Petroleum Institute. Research Project 44; Selected ...
-114.14	CRC Handbook of Chemistry and Physics
-114.10	DrugBank
-114.40	Merck Index
-114.00	Oxford University MSDS
-114.10	PHYSPROP
-114.00	Sigma-Aldrich
-114.30	Wikipedia
	Values not used in calculating the average melting point
-130.00	Alfa Aesar[1]
-144.00	Oxford University MSDS[2]

1. confirmed error with source JCB
2. clearly out of range JCB

ethofenprox C25H28O3[61, 64]



Compound Data

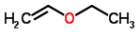
Melting point	**36.50 °C**	**309.65 K**			
CSID	64377	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	376.488	**H bond donors**	0	**ACD/LogP**	7.34
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.07 g/cm^3
SMILES	O(c1ccccc1)c2cc(ccc2)COCC(c3ccc(OCC)cc3)(C)C				

STD InChIKey	YREQHYQNNWYQCJ-UHFFFAOYAW

Melting Points

mp °C	source
36.00	Oxford University MSDS
37.00	PHYSPROP

ethoxyethene C4H8O[3, 61, 64]



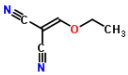
Compound Data

Melting point	**-115.27 °C**	**157.88 K**			
CSID	7732	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	72.1057	**H bond donors**	0	**ACD/LogP**	1.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.75 g/cm^3
SMILES	O(\C=C)CC				
STD InChIKey	FJKIXWOMBXYWOQ-UHFFFAOYAE				

Melting Points

mp °C	source
-115.00	Alfa Aesar
-115.00	Oxford University MSDS
-115.80	PHYSPROP

ethoxymethylenemalononitrile C6H6N2O[3, 64]



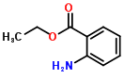
Compound Data

Melting point	**65.50 °C**	**338.65 K**			
CSID	60497	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	122.1246	**H bond donors**	0	**ACD/LogP**	0.31
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.07 g/cm^3
SMILES	N#C/C(C#N)=C\OCC				
STD InChIKey	OEICGMPRFOJHKO-UHFFFAOYAG				

Melting Points

mp °C	source
65.00	Alfa Aesar
66.00	PHYSPROP

ethyl 2-aminobenzoate C9H11NO2[2, 3, 61, 64]



Compound Data

Melting point	**13.75 °C**	**286.90 K**			
CSID	21106112	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	165.1891	**H bond donors**	2	**ACD/LogP**	2.57
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	O=C(OCC)c1ccccc1N				
STD InChIKey	TWLLPUMZVVGILS-UHFFFAOYAR				

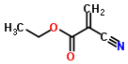
Melting Points

mp °C	source
14.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
15.00	Alfa Aesar
13.00	Oxford University MSDS
13.00	PHYSPROP

ethyl 2-cyanoacrylate C6H7NO2[61, 64]

Compound Data

Melting point	**-22.25 °C**	**250.90 K**			
CSID	73564	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	125.1253	**H bond donors**	0	**ACD/LogP**	0.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3



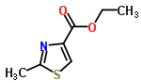
SMILES	N#C/C(=C)C(=O)OCC
STD InChIKey	FGBJXOREULPLGL-UHFFFAOYAG

Melting Points

mp °C	source
-22.00	Oxford University MSDS
-22.50	PHYSPROP

ethyl 2-methylthiazole-4-carboxylate C7H9NO2S[3, 48]

Compound Data



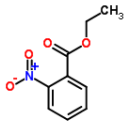
Melting point	**56.00 °C**	**329.15 K**			
CSID	258907	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.2169	**H bond donors**	0	**ACD/LogP**	1.44
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.20 g/cm^3
SMILES	CCOC(=O)c1csc(n1)C				
STD InChIKey	QWWPUBQHZFHZSF-UHFFFAOYAZ				

Melting Points

mp °C	source
55.00	Alfa Aesar
57.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

ethyl 2-nitrobenzoate C9H9NO4[3, 64]

Compound Data



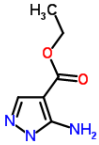
Melting point	**29.00 °C**	**302.15 K**			
CSID	62340	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	195.1721	**H bond donors**	0	**ACD/LogP**	2.19
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=[N+]([O-])c1ccccc1C(=O)OCC				
STD InChIKey	CPNMAYYYYSWTIV-UHFFFAOYAJ				

Melting Points

mp °C	source
28.00	Alfa Aesar
30.00	PHYSPROP

ethyl 3-aminopyrazole-4-carboxylate C6H9N3O2[3, 48]

Compound Data



Melting point	**104.50 °C**	**377.65 K**			
CSID	73512	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	155.1546	**H bond donors**	3	**ACD/LogP**	0.67
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.32 g/cm^3
SMILES	O=C(OCC)c1cnnc1N				
STD InChIKey	YPXGHKWOJXQLQU-UHFFFAOYAP				

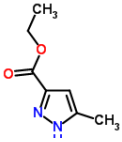
Melting Points

mp °C	source
106.00	Alfa Aesar
103.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

ethyl 3-methylpyrazole-5-carboxylate C7H10N2O2[3, 48, 48]

Compound Data

Melting point	**83.67 °C**	**356.82 K**			
CSID	70048	**H bond acceptors**	4	**Rule of 5 violations**	0



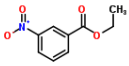
Molecular weight	154.1665	**H bond donors**	1	**ACD/LogP**	1.29
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OCC)c1nnc(c1)C				
STD InChIKey	BOTXQJAHRCGJEG-UHFFFAOYAW				

Melting Points

mp °C	source
82.00	Alfa Aesar
82.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
87.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

ethyl 3-nitrobenzoate C9H9NO4[3, 64]

Compound Data



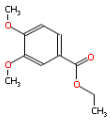
Melting point	**44.50 °C**	**317.65 K**			
CSID	21106111	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	195.1721	**H bond donors**	0	**ACD/LogP**	2.35
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1)C(=O)OCC				
STD InChIKey	MKBIJCPQTPFQKQ-UHFFFAOYAR				

Melting Points

mp °C	source
42.00	Alfa Aesar
47.00	PHYSPROP

ethyl 3,4-dimethoxybenzoate C11H14O4[3, 64]

Compound Data



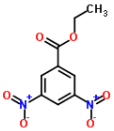
Melting point	**43.75 °C**	**316.90 K**			
CSID	21171999	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	210.2265	**H bond donors**	0	**ACD/LogP**	2.59
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.09 g/cm^3
SMILES	COc1cc(ccc1OC)C(=O)OCC				
STD InChIKey	AYYNUGSDPRDVCH-UHFFFAOYAS				

Melting Points

mp °C	source
44.00	Alfa Aesar
43.50	PHYSPROP

ethyl 3,5-dinitrobenzoate C9H8N2O6[3, 64]

Compound Data



Melting point	**93.00 °C**	**366.15 K**			
CSID	62468	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	240.1696	**H bond donors**	0	**ACD/LogP**	1.91
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.43 g/cm^3
SMILES	O=[N+]([O-])c1cc(cc([N+]([O-])=O)c1)C(=O)OCC				
STD InChIKey	IBQREHJPMPCXQA-UHFFFAOYAK				

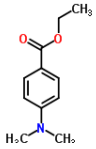
Melting Points

mp °C	source
92.00	Alfa Aesar
94.00	PHYSPROP

ethyl 4-(dimethylamino)benzoate C11H15NO2[3, 61]

Compound Data

Melting point	**63.75 °C**	**336.90 K**	



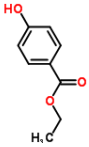
CSID	23472	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	193.2423	**H bond donors**	0	**ACD/LogP**	3.14
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.06 g/cm^3
SMILES	O=C(OCC)c1ccc(N(C)C)cc1				
STD InChIKey	FZUGPQWGEGAKET-UHFFFAOYAL				

Melting Points

mp °C	source
64.00	Alfa Aesar
63.50	Oxford University MSDS

ethyl 4-hydroxybenzoate C9H10O3[3, 44, 61, 64]

Compound Data



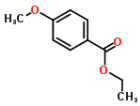
Melting point	**116.75 °C**	**389.90 K**			
CSID	13846749	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OCC)c1ccc(O)cc1				
STD InChIKey	NUVBSKCKDOMJSU-UHFFFAOYAQ				

Melting Points

mp °C	source
117.00	Alfa Aesar
116.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
117.00	Oxford University MSDS
117.00	PHYSPROP

ethyl 4-methoxybenzoate C10H12O3[3, 7, 64]

Compound Data



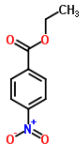
Melting point	**7.50 °C**	**280.65 K**			
CSID	21159425	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	0	**ACD/LogP**	2.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.07 g/cm^3
SMILES	COc1ccc(cc1)C(=O)OCC				
STD InChIKey	FHUODBDRWMIBQP-UHFFFAOYAR				

Melting Points

mp °C	source
8.00	Alfa Aesar
7.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
7.50	PHYSPROP

ethyl 4-nitrobenzoate C9H9NO4[2, 3, 64]

Compound Data

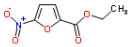


Melting point	**57.33 °C**	**330.48 K**			
CSID	7177	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	195.1721	**H bond donors**	0	**ACD/LogP**	2.33
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C(=O)OCC)cc1				
STD InChIKey	PHWSCBWNPZDYRI-UHFFFAOYAV				

Melting Points

mp °C	source
58.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
57.00	Alfa Aesar
57.00	PHYSPROP

ethyl 5-nitro-2-furoate C7H7NO5[3, 48]



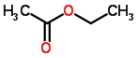
Compound Data

Melting point	**100.50 °C**	**373.65 K**			
CSID	63522	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	185.1342	**H bond donors**	0	**ACD/LogP**	0.81
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.34 g/cm^3
SMILES	O=C(OCC)c1oc([N+](=O)[O-])cc1				
STD InChIKey	JMNXLAQKIHVFIC-UHFFFAOYAA				

Melting Points

mp °C	source
100.00	Alfa Aesar
101.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

ethyl acetate C4H8O2[2, 3, 61, 64]



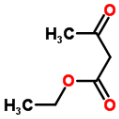
Compound Data

Melting point	**-83.90 °C**	**189.25 K**			
CSID	8525	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	0	**ACD/LogP**	0.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.90 g/cm^3
SMILES	O=C(OCC)C				
STD InChIKey	XEKOWRVHYACXOJ-UHFFFAOYAD				

Melting Points

mp °C	source
-84.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-84.00	Alfa Aesar
-84.00	Oxford University MSDS
-83.60	PHYSPROP

ethyl acetoacetate C6H10O3[2, 3, 61, 64]



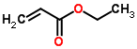
Compound Data

Melting point	**-43.50 °C**	**229.65 K**			
CSID	13865426	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	130.1418	**H bond donors**	0	**ACD/LogP**	0.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.01 g/cm^3
SMILES	CCOC(=O)CC(=O)C				
STD InChIKey	XYIBRDXRRQCHLP-UHFFFAOYAP				

Melting Points

mp °C	source
-43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-43.00	Alfa Aesar
-43.00	Oxford University MSDS
-45.00	PHYSPROP

ethyl acrylate C5H8O2[2, 3, 61, 64]



Compound Data

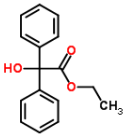
Melting point	**-71.05 °C**	**202.10 K**			
CSID	8490	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1158	**H bond donors**	0	**ACD/LogP**	1.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.91 g/cm^3
SMILES	CCOC(=O)C=C				
STD InChIKey	JIGUQPWFLRLWPJ-UHFFFAOYAN				

Melting Points

mp °C	source
-71.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-71.00	Alfa Aesar
-71.00	Oxford University MSDS

-71.20	PHYSPROP

ethyl benzilate C16H16O3[3, 64]



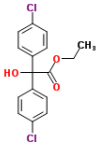
Compound Data

Melting point	**32.00 °C**	**305.15 K**			
CSID	86894	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	256.2964	**H bond donors**	1	**ACD/LogP**	3.54
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.16 g/cm^3
SMILES	O=C(OCC)C(O)(c1ccccc1)c2ccccc2				
STD InChIKey	AIPVNQQMYPWQSX-UHFFFAOYAG				

Melting Points

mp °C	source
30.00	Alfa Aesar
34.00	PHYSPROP

ethyl bis(4-chlorophenyl)(hydroxy)acetate C16H14Cl2O3[61, 64]



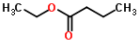
Compound Data

Melting point	**36.50 °C**	**309.65 K**			
CSID	10085	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	325.1866	**H bond donors**	1	**ACD/LogP**	4.73
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.33 g/cm^3
SMILES	Clc1ccc(cc1)C(O)(c2ccc(Cl)cc2)C(=O)OCC				
STD InChIKey	RAPBNVDSDCTNRC-UHFFFAOYAH				

Melting Points

mp °C	source
36.00	Oxford University MSDS
37.00	PHYSPROP

ethyl butyrate C6H12O2[2, 3, 61, 64]



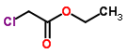
Compound Data

Melting point	**-94.25 °C**	**178.90 K**			
CSID	7475	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	0	**ACD/LogP**	1.80
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.89 g/cm^3
SMILES	CCCC(=O)OCC				
STD InChIKey	OBNCKNCVKJNDBV-UHFFFAOYAO				

Melting Points

mp °C	source
-93.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-93.00	Alfa Aesar
-93.00	Oxford University MSDS
-98.00	PHYSPROP

ethyl chloroacetate C4H7ClO2[3, 61, 64]



Compound Data

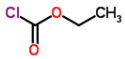
Melting point	**-24.33 °C**	**248.82 K**			
CSID	7465	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.5502	**H bond donors**	0	**ACD/LogP**	0.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.12 g/cm^3
SMILES	ClCC(=O)OCC				
STD InChIKey	VEUUMBGHMNQHGO-UHFFFAOYAS				

Melting Points

mp °C	source
-26.00	Alfa Aesar

-26.00	Oxford University MSDS
-21.00	PHYSPROP

ethyl chloroformate C3H5ClO2[3, 64]



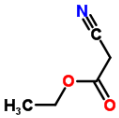
Compound Data

Melting point	**-80.80 °C**	**192.35 K**			
CSID	10465	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.5236	**H bond donors**	0	**ACD/LogP**	1.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	ClC(=O)OCC				
STD InChIKey	RIFGWPKJUGCATF-UHFFFAOYAX				

Melting Points

mp °C	source
-81.00	Alfa Aesar
-80.60	PHYSPROP

ethyl cyanoacetate C5H7NO2[2, 3, 64]



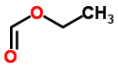
Compound Data

Melting point	**-22.50 °C**	**250.65 K**			
CSID	13856579	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	113.1146	**H bond donors**	0	**ACD/LogP**	0.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3
SMILES	N#CCC(=O)OCC				
STD InChIKey	ZIUSEGSNTOUIPT-UHFFFAOYAI				

Melting Points

mp °C	source
-22.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-23.00	Alfa Aesar
-22.50	PHYSPROP

ethyl formate C3H6O2[2, 3, 61, 64]



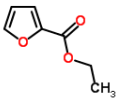
Compound Data

Melting point	**-80.40 °C**	**192.75 K**			
CSID	7734	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	74.0785	**H bond donors**	0	**ACD/LogP**	0.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.91 g/cm^3
SMILES	O=COCC				
STD InChIKey	WBJINCZRORDGAQ-UHFFFAOYAO				

Melting Points

mp °C	source
-80.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-81.00	Alfa Aesar
-81.00	Oxford University MSDS
-79.60	PHYSPROP

ethyl furoate C7H8O3[3, 64]



Compound Data

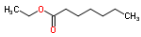
Melting point	**34.25 °C**	**307.40 K**			
CSID	11485	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	140.1366	**H bond donors**	0	**ACD/LogP**	1.52
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=C(OCC)c1occc1				
STD InChIKey	NHXSTXWKZVAVOQ-UHFFFAOYAN				

Melting Points

mp °C	source
34.00	Alfa Aesar
34.50	PHYSPROP

ethyl heptanoate C9H18O2[3, 7, 64]

Compound Data



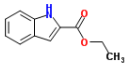
Melting point	**-66.03 °C**	**207.12 K**			
CSID	7509	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.238	**H bond donors**	0	**ACD/LogP**	3.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCC)CCCCCC				
STD InChIKey	TVQGDYNRXLTQAP-UHFFFAOYAW				

Melting Points

mp °C	source
-66.00	Alfa Aesar
-66.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
-66.10	PHYSPROP

ethyl indole-2-carboxylate C11H11NO2[3, 64]

Compound Data



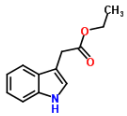
Melting point	**123.75 °C**	**396.90 K**			
CSID	65903	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	189.2105	**H bond donors**	1	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	O=C(OCC)c2cc1ccccc1n2				
STD InChIKey	QQXQAEWRSVZPJM-UHFFFAOYAR				

Melting Points

mp °C	source
124.00	Alfa Aesar
123.50	PHYSPROP

ethyl indole-3-acetate C12H13NO2[3, 64]

Compound Data



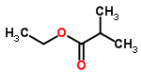
Melting point	**43.75 °C**	**316.90 K**			
CSID	12523	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	203.2371	**H bond donors**	1	**ACD/LogP**	2.42
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.19 g/cm^3
SMILES	O=C(OCC)Cc2c1ccccc1nc2				
STD InChIKey	HUDBDWIQSIGUDI-UHFFFAOYAQ				

Melting Points

mp °C	source
43.00	Alfa Aesar
44.50	PHYSPROP

ethyl isobutyrate C6H12O2[3, 64]

Compound Data



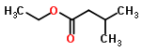
Melting point	**-88.10 °C**	**185.05 K**			
CSID	7065	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	0	**ACD/LogP**	1.59
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCC)C(C)C				
STD InChIKey	WDAXFOBOLVPGLV-UHFFFAOYAG				

Melting Points

mp °C	source

-88.00	Alfa Aesar
-88.20	PHYSPROP

ethyl isovalerate C7H14O2[2, 3, 64]



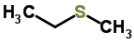
Compound Data

Melting point	**-99.10 °C**	**174.05 K**			
CSID	7657	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1849	**H bond donors**	0	**ACD/LogP**	2.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCC)CC(C)C				
STD InChIKey	PPXUHEORWJQRHJ-UHFFFAOYAE				

Melting Points

mp °C	source
-99.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-99.00	Alfa Aesar
-99.30	PHYSPROP

ethyl methyl sulfide C3H8S[3, 4, 64]



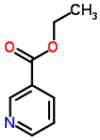
Compound Data

Melting point	**-105.97 °C**	**167.18 K**			
CSID	11729	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	76.1606	**H bond donors**	0	**ACD/LogP**	1.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.83 g/cm^3
SMILES	S(CC)C				
STD InChIKey	WXEHBUMAEPOYKP-UHFFFAOYAC				

Melting Points

mp °C	source
-106.00	Alfa Aesar
-106.00	American Petroleum Institute. Research Project 44; Selected ...
-105.90	PHYSPROP

ethyl nicotinate C8H9NO2[3, 64]



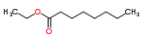
Compound Data

Melting point	**8.75 °C**	**281.90 K**			
CSID	62402	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	0	**ACD/LogP**	1.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(OCC)c1cccnc1				
STD InChIKey	XBLVHTDFJBKJLG-UHFFFAOYAV				

Melting Points

mp °C	source
9.00	Alfa Aesar
8.50	PHYSPROP

ethyl octanoate C10H20O2[2, 3, 64]



Compound Data

Melting point	**-45.70 °C**	**227.45 K**			
CSID	7511	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.2646	**H bond donors**	0	**ACD/LogP**	3.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.87 g/cm^3
SMILES	O=C(OCC)CCCCCCC				
STD InChIKey	YYZUSRORWSJGET-UHFFFAOYAU				

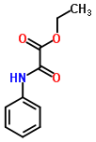
Melting Points

mp °C	source

-47.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-47.00	Alfa Aesar
-43.10	PHYSPROP

ethyl oxanilate C10H11NO3[3, 64]

Compound Data



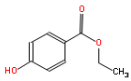
Melting point	**66.25 °C**	**339.40 K**			
CSID	66460	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	193.1992	**H bond donors**	1	**ACD/LogP**	1.48
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.22 g/cm^3
SMILES	O=C(Nc1ccccc1)C(=O)OCC				
STD InChIKey	YDGAUBHNAKCSKF-UHFFFAOYAA				

Melting Points

mp °C	source
67.00	Alfa Aesar
65.50	PHYSPROP

ethyl p-hydroxybenzoate C9H10O3[70, 72]

Compound Data



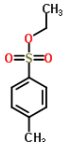
Melting point	**115.75 °C**	**388.90 K**			
CSID	8127	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	1	**ACD/LogP**	2.40
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OCC)c1ccc(O)cc1				
STD InChIKey	NUVBSKCKDOMJSU-UHFFFAOYSA-N				

Melting Points

mp °C	source
116.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
115.50	Sigma-Aldrich

ethyl p-toluenesulfonate C9H12O3S[2, 3, 64]

Compound Data



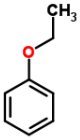
Melting point	**33.50 °C**	**306.65 K**			
CSID	6386	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	200.2548	**H bond donors**	0	**ACD/LogP**	1.83
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3
SMILES	O=S(=O)(OCC)c1ccc(cc1)C				
STD InChIKey	VRZVPALEJCLXPR-UHFFFAOYAO				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar
34.50	PHYSPROP

ethyl phenyl ether C8H10O[2, 3, 64]

Compound Data



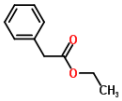
Melting point	**-29.83 °C**	**243.32 K**			
CSID	7391	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	122.1644	**H bond donors**	0	**ACD/LogP**	2.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.94 g/cm^3
SMILES	O(c1ccccc1)CC				
STD InChIKey	DLRJIFUOBPOJNS-UHFFFAOYAS				

Melting Points

mp °C	source

-30.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-30.00	Alfa Aesar
-29.50	PHYSPROP

ethyl phenylacetate C10H12O2[3, 64]



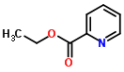
Compound Data

Melting point	**-29.20 °C**	**243.95 K**			
CSID	13885245	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	0	**ACD/LogP**	2.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.03 g/cm^3
SMILES	O=C(Cc1ccccc1)OCC				
STD InChIKey	DULCUDSUACXJJC-UHFFFAOYAN				

Melting Points

mp °C	source
-29.00	Alfa Aesar
-29.40	PHYSPROP

ethyl picolinate C8H9NO2[3, 64]



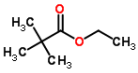
Compound Data

Melting point	**1.50 °C**	**274.65 K**			
CSID	16377	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	0	**ACD/LogP**	1.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(OCC)c1ncccc1				
STD InChIKey	FQYYIPZPELSLDK-UHFFFAOYAQ				

Melting Points

mp °C	source
2.00	Alfa Aesar
1.00	PHYSPROP

ethyl pivalate C7H14O2[3, 64]



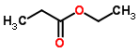
Compound Data

Melting point	**-89.75 °C**	**183.40 K**			
CSID	18688	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1849	**H bond donors**	0	**ACD/LogP**	1.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCC)C(C)(C)C				
STD InChIKey	HHEIMYAXCOIQCJ-UHFFFAOYAH				

Melting Points

mp °C	source
-90.00	Alfa Aesar
-89.50	PHYSPROP

ethyl propionate C5H10O2[2, 3, 64]



Compound Data

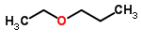
Melting point	**-73.30 °C**	**199.85 K**			
CSID	7463	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	0	**ACD/LogP**	1.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.89 g/cm^3
SMILES	O=C(OCC)CC				
STD InChIKey	FKRCODPIKNYEAC-UHFFFAOYAW				

Melting Points

mp °C	source
-73.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

-73.00	Alfa Aesar
-73.90	PHYSPROP

ethyl propyl ether C5H12O[4, 64]



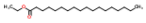
Compound Data

Melting point	**-127.25 °C**	**145.90 K**			
CSID	11835	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	0	**ACD/LogP**	1.51
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.75 g/cm^3
SMILES	O(CC)CCC				
STD InChIKey	NVJUHMXYKCUMQA-UHFFFAOYAW				

Melting Points

mp °C	source
-127.00	American Petroleum Institute. Research Project 44; Selected ...
-127.50	PHYSPROP

ethyl stearate C20H40O2[3, 64]



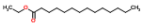
Compound Data

Melting point	**34.00 °C**	**307.15 K**			
CSID	7830	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	312.5304	**H bond donors**	0	**ACD/LogP**	9.21
Phase 25 °C	solid	**Rotatable bonds**	18	**Predicted density**	0.86 g/cm^3
SMILES	O=C(OCC)CCCCCCCCCCCCCCCCC				
STD InChIKey	MVLVMROFTAUDAG-UHFFFAOYAC				

Melting Points

mp °C	source
35.00	Alfa Aesar
33.00	PHYSPROP

ethyl tetradecanoate C16H32O2[3, 64]



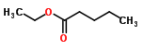
Compound Data

Melting point	**12.15 °C**	**285.30 K**			
CSID	29023	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	256.4241	**H bond donors**	0	**ACD/LogP**	7.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	0.86 g/cm^3
SMILES	O=C(OCC)CCCCCCCCCCCCC				
STD InChIKey	MMKRHZKQPFCLLS-UHFFFAOYAA				

Melting Points

mp °C	source
12.00	Alfa Aesar
12.30	PHYSPROP

ethyl valerate C7H14O2[3, 64]



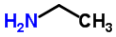
Compound Data

Melting point	**-91.10 °C**	**182.05 K**			
CSID	10420	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1849	**H bond donors**	0	**ACD/LogP**	2.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCC)CCCC				
STD InChIKey	ICMAFTSLXCXHRK-UHFFFAOYAC				

Melting Points

mp °C	source
-91.00	Alfa Aesar
-91.20	PHYSPROP

ethylamine C_2H_7N[61, 64]



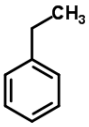
Compound Data

Melting point	**-81.10 °C**	**192.05 K**			
CSID	6101	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	45.0837	**H bond donors**	2	**ACD/LogP**	-0.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.69 g/cm^3
SMILES	NCC				
STD InChIKey	QUSNBJAOOMFDIB-UHFFFAOYAL				

Melting Points

mp °C	source
-81.00	Oxford University MSDS
-81.20	PHYSPROP

ethylbenzene C_8H_{10}[3, 4, 32, 64]



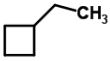
Compound Data

Melting point	**-94.95 °C**	**178.20 K**			
CSID	7219	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	106.165	**H bond donors**	0	**ACD/LogP**	3.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.87 g/cm^3
SMILES	CCc1ccccc1				
STD InChIKey	YNQLUTRBYVCPMQ-UHFFFAOYAM				

Melting Points

mp °C	source
-95.00	Alfa Aesar
-95.00	American Petroleum Institute. Research Project 44; Selected ...
-94.90	DrugBank
-94.90	PHYSPROP

ethylcyclobutane C_6H_{12}[4, 64]



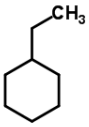
Compound Data

Melting point	**-142.95 °C**	**130.20 K**			
CSID	221079	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.78 g/cm^3
SMILES	CCC1CCC1				
STD InChIKey	NEZRFXZYPAIZAD-UHFFFAOYAY				

Melting Points

mp °C	source
-143.00	American Petroleum Institute. Research Project 44; Selected ...
-142.90	PHYSPROP

ethylcyclohexane C_8H_{16}[4, 64]



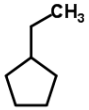
Compound Data

Melting point	**-111.15 °C**	**162.00 K**			
CSID	14751	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.78 g/cm^3
SMILES	CCC1CCCCC1				
STD InChIKey	IIEWJVIFRVWJOD-UHFFFAOYAU				

Melting Points

mp °C	source
-111.00	American Petroleum Institute. Research Project 44; Selected ...
-111.30	PHYSPROP

ethylcyclopentane C7H14[4, 64]



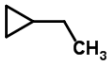
Compound Data

Melting point	**-138.20 °C**	**134.95 K**			
CSID	14686	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.85
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.78 g/cm^3
SMILES	CCC1CCCC1				
STD InChIKey	IFTRQJLVEBNKJK-UHFFFAOYAM				

Melting Points

mp °C	source
-138.00	American Petroleum Institute. Research Project 44; Selected ...
-138.40	PHYSPROP

ethylcyclopropane C5H10[4, 64]



Compound Data

Melting point	**-149.10 °C**	**124.05 K**			
CSID	64095	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.1329	**H bond donors**	0	**ACD/LogP**	2.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.77 g/cm^3
SMILES	CCC1CC1				
STD InChIKey	FOTXAJDDGPYIFU-UHFFFAOYAR				

Melting Points

mp °C	source
-149.00	American Petroleum Institute. Research Project 44; Selected ...
-149.20	PHYSPROP

ethylene C2H4[60, 61, 64, 73]

Compound Data

Melting point	**-169.14 °C**	**104.01 K**			
CSID	6085	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	28.0532	**H bond donors**	0	**ACD/LogP**	1.32
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.48 g/cm^3
SMILES	C=C				
STD InChIKey	VGGSQFUCUMXWEO-UHFFFAOYAE				

Melting Points

mp °C	source
-169.20	Oka T; Sato S. Bulletin of the Chemical Society of Japan 42(...
-169.00	Oxford University MSDS
-169.00	PHYSPROP
-169.35	Streng AG Journal of Chemical and Engineering Data 16(3) 357...

ethylene oxide C2H4O[61, 64]

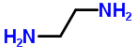
Compound Data

Melting point	**-111.35 °C**	**161.80 K**			
CSID	6114	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	44.0526	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.99 g/cm^3
SMILES	C1CO1				
STD InChIKey	IAYPIBMASNFSPL-UHFFFAOYAX				

Melting Points

mp °C	source
-111.00	Oxford University MSDS
-111.70	PHYSPROP

ethylenediamine $C_2H_8N_2$[3, 61, 64]



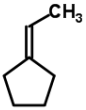
Compound Data

Melting point	**9.87 °C**	**283.02 K**			
CSID	13835550	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	60.0983	**H bond donors**	4	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.87 g/cm^3
SMILES	C(CN)N				
STD InChIKey	PIICEJLVQHRZGT-UHFFFAOYAH				

Melting Points

mp °C	source
10.00	Alfa Aesar
8.50	Oxford University MSDS
11.10	PHYSPROP

ethylidenecyclopentane C_7H_{12}[3, 64]



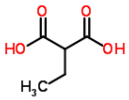
Compound Data

Melting point	**-129.75 °C**	**143.40 K**			
CSID	67620	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1702	**H bond donors**	0	**ACD/LogP**	3.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.91 g/cm^3
SMILES	C(=C1/CCCC1)\C				
STD InChIKey	VONKRKBGTZDZNV-UHFFFAOYAN				

Melting Points

mp °C	source
-130.00	Alfa Aesar
-129.50	PHYSPROP

ethylmalonic acid $C_5H_8O_4$[3, 64]



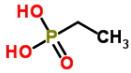
Compound Data

Melting point	**113.50 °C**	**386.65 K**			
CSID	11263	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	132.1146	**H bond donors**	2	**ACD/LogP**	0.32
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.31 g/cm^3
SMILES	O=C(O)C(C(=O)O)CC				
STD InChIKey	UKFXDFUAPNAMPJ-UHFFFAOYAZ				

Melting Points

mp °C	source
113.00	Alfa Aesar
114.00	PHYSPROP

ethylphosphonic acid $C_2H_7O_3P$[3, 61]



Compound Data

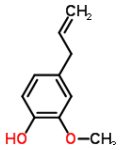
Melting point	**60.75 °C**	**333.90 K**			
CSID	177126	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	110.0489	**H bond donors**	2	**ACD/LogP**	-1.49
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	O=P(O)(O)CC				
STD InChIKey	GATNOFPXSDHULC-UHFFFAOYAH				

Melting Points

mp °C	source
60.00	Alfa Aesar
61.50	Oxford University MSDS

eugenol C10H12O2[3, 61, 64]

Compound Data



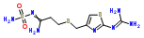
Melting point	**-9.37 °C**	**263.78 K**			
CSID	13876103	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2011	**H bond donors**	1	**ACD/LogP**	2.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.05 g/cm^3
SMILES	Oc1ccc(cc1OC)CC=C				
STD InChIKey	RRAFCDWBNXTKKO-UHFFFAOYAJ				

Melting Points

mp °C	source
-10.00	Alfa Aesar
-9.00	Oxford University MSDS
-9.10	PHYSPROP

famotidine C8H15N7O2S3[9, 32, 44, 64]

Compound Data



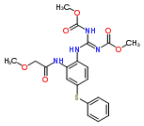
Melting point	**163.38 °C**	**436.52 K**			
CSID	3208	**H bond acceptors**	9	**Rule of 5 violations**	1
Molecular weight	337.4454	**H bond donors**	8	**ACD/LogP**	-0.40
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.83 g/cm^3
SMILES	O=S(=O)(N=C(N)CCSCc1nc(/N=C(/N)N)sc1)N				
STD InChIKey	XUFQPHANEAPEMJ-UHFFFAOYAG				

Melting Points

mp °C	source
163.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
163.50	DrugBank
163.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
163.50	PHYSPROP

febantel C20H22N4O6S[9, 48, 64]

Compound Data



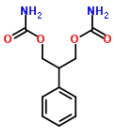
Melting point	**129.17 °C**	**402.32 K**			
CSID	4514715	**H bond acceptors**	10	**Rule of 5 violations**	1
Molecular weight	446.4769	**H bond donors**	3	**ACD/LogP**	2.79
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.31 g/cm^3
SMILES	O=C(OC)N/C(=N\C(=O)OC)Nc2c(cc(Sc1ccccc1)cc2)NC(=O)COC				
STD InChIKey	HMCCXLBXIJMERM-UHFFFAOYAA				

Melting Points

mp °C	source
129.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
129.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
129.50	PHYSPROP

felbamate C11H14N2O4[9, 32, 48, 64]

Compound Data



Melting point	**151.38 °C**	**424.52 K**			
CSID	3214	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	238.2399	**H bond donors**	4	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.27 g/cm^3
SMILES	O=C(OCC(c1ccccc1)COC(=O)N)N				
STD InChIKey	WKGXYQFOCVYPAC-UHFFFAOYAJ				

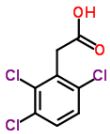
Melting Points

mp °C	source
151.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
151.50	DrugBank

151.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
152.00	PHYSPROP

fenac C8H5Cl3O2[61, 64]

Compound Data



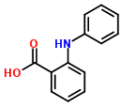
Melting point	**158.50 °C**	**431.65 K**			
CSID	6546	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	239.4831	**H bond donors**	1	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.57 g/cm^3
SMILES	Clc1c(c(Cl)ccc1Cl)CC(=O)O				
STD InChIKey	QZXCCPZJCKEPSA-UHFFFAOYAP				

Melting Points

mp °C	source
156.00	Oxford University MSDS
161.00	PHYSPROP

fenamic acid C13H11NO2[3, 64]

Compound Data



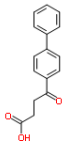
Melting point	**185.25 °C**	**458.40 K**			
CSID	4233	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	213.2319	**H bond donors**	2	**ACD/LogP**	4.41
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	O=C(O)c2ccccc2Nc1ccccc1				
STD InChIKey	ZWJINEZUASEZBH-UHFFFAOYAQ				

Melting Points

mp °C	source
187.00	Alfa Aesar
183.50	PHYSPROP

fenbufen C16H14O3[44, 64]

Compound Data



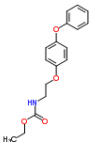
Melting point	**186.05 °C**	**459.20 K**			
CSID	3218	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	254.2806	**H bond donors**	1	**ACD/LogP**	3.13
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.19 g/cm^3
SMILES	O=C(O)CCC(=O)c2ccc(c1ccccc1)cc2				
STD InChIKey	ZPAKPRAICRBAOD-UHFFFAOYAO				

Melting Points

mp °C	source
186.10	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
186.00	PHYSPROP

fenoxycarb C17H19NO4[44, 64, 64]

Compound Data



Melting point	**53.33 °C**	**326.48 K**			
CSID	46739	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	301.3371	**H bond donors**	1	**ACD/LogP**	3.83
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.15 g/cm^3
SMILES	O=C(OCC)NCCOc2ccc(Oc1ccccc1)cc2				
STD InChIKey	HJUFTIJOISQSKQ-UHFFFAOYAM				

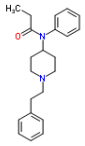
Melting Points

mp °C	source
53.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
53.00	PHYSPROP

53.50	PHYSPROP

fentanyl C22H28N2O[9, 48, 64]

Compound Data



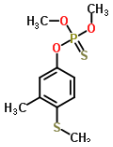
Melting point	**84.50 °C**	**357.65 K**			
CSID	3228	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	336.4705	**H bond donors**	0	**ACD/LogP**	3.89
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.09 g/cm^3
SMILES	O=C(N(c1ccccc1)C3CCN(CCc2ccccc2)CC3)CC				
STD InChIKey	PJMPHNIQZUBGLI-UHFFFAOYAZ				

Melting Points

mp °C	source
83.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
83.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
87.50	PHYSPROP

fenthion C10H15O3PS2[61, 64]

Compound Data



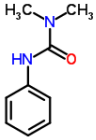
Melting point	**7.25 °C**	**280.40 K**			
CSID	3229	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	278.3281	**H bond donors**	0	**ACD/LogP**	3.21
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.25 g/cm^3
SMILES	S=P(OC)(OC)Oc1ccc(SC)c(c1)C				
STD InChIKey	PNVJTZOFSHSLTO-UHFFFAOYAH				

Melting Points

mp °C	source
7.00	Oxford University MSDS
7.50	PHYSPROP

fenuron C9H12N2O[64, 70, 70]

Compound Data



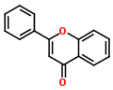
Melting point	**133.83 °C**	**406.98 K**			
CSID	7279	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	164.2044	**H bond donors**	1	**ACD/LogP**	0.98
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.12 g/cm^3
SMILES	O=C(Nc1ccccc1)N(C)C				
STD InChIKey	XXOYNJXVWVNOOJ-UHFFFAOYAE				

Melting Points

mp °C	source
133.50	PHYSPROP
134.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
134.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

flavone C15H10O2[3, 64]

Compound Data



Melting point	**98.50 °C**	**371.65 K**			
CSID	10230	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	222.2387	**H bond donors**	0	**ACD/LogP**	3.56
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	O=C\1c3c(O/C(=C/1)c2ccccc2)cccc3				
STD InChIKey	VHBFFQKBGNRLFZ-UHFFFAOYAG				

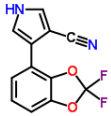
Melting Points

mp °C	source
97.00	Alfa Aesar

100.00	PHYSPROP

fludioxonil C12H6F2N2O2[44, 64]

Compound Data



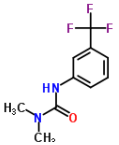
Melting point	**199.60 °C**	**472.75 K**			
CSID	77916	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	248.185	**H bond donors**	1	**ACD/LogP**	3.62
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.55 g/cm^3
SMILES	N#Cc3cncc3c1cccc2OC(F)(F)Oc12				
STD InChIKey	MUJOIMFVNIBMKC-UHFFFAOYAI				

Melting Points

mp °C	source
199.40	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
199.80	PHYSPROP

fluometuron C10H11F3N2O[44, 64]

Compound Data



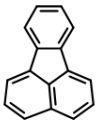
Melting point	**163.75 °C**	**436.90 K**			
CSID	15702	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	232.2023	**H bond donors**	1	**ACD/LogP**	2.36
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	O=C(Nc1cc(ccc1)C(F)(F)F)N(C)C				
STD InChIKey	RZILCCPWPBTYDO-UHFFFAOYAP				

Melting Points

mp °C	source
163.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
164.00	PHYSPROP

fluoranthene C16H10[61, 64, 70]

Compound Data



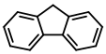
Melting point	**107.77 °C**	**380.92 K**			
CSID	8800	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	202.2506	**H bond donors**	0	**ACD/LogP**	5.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	c1ccc-2c(c1)-c3cccc4c3c2ccc4				
STD InChIKey	GVEPBJHOBDJJJI-UHFFFAOYAL				

Melting Points

mp °C	source
107.50	Oxford University MSDS
107.80	PHYSPROP
108.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

fluorene C13H10[2, 3, 44, 48, 61, 64, 70]

Compound Data



Melting point	**114.90 °C**	**388.05 K**			
CSID	6592	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	166.2185	**H bond donors**	0	**ACD/LogP**	4.32
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.12 g/cm^3
SMILES	c1ccc-2c(c1)Cc3c2cccc3				
STD InChIKey	NIHNNTQXNPWCJQ-UHFFFAOYAW				

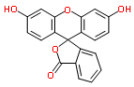
Melting Points

mp °C	source
114.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
115.00	Alfa Aesar

116.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
116.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
116.00	Oxford University MSDS
114.80	PHYSPROP
112.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

fluorescein C20H12O5[3, 32]

Compound Data



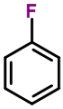
Melting point	**317.50 °C**	**590.65 K**			
CSID	15968	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	332.3063	**H bond donors**	2	**ACD/LogP**	2.68
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.60 g/cm^3
SMILES	c1ccc2c(c1)C(=O)OC23c4ccc(cc4Oc5c3ccc(c5)O)O				
STD InChIKey	GNBHRKFJIUUOQI-UHFFFAOYAZ				

Melting Points

mp °C	source
320.00	Alfa Aesar
315.00	DrugBank

fluorobenzene C6H5F[3, 61, 64]

Compound Data



Melting point	**-41.40 °C**	**231.75 K**			
CSID	9614	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	96.1023	**H bond donors**	0	**ACD/LogP**	2.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.03 g/cm^3
SMILES	Fc1ccccc1				
STD InChIKey	PYLWMHQQBFSUBP-UHFFFAOYAM				

Melting Points

mp °C	source
-42.00	Alfa Aesar
-40.00	Oxford University MSDS
-42.20	PHYSPROP

fluoroform CHF3[61, 64]

Compound Data

Melting point	**-157.55 °C**	**115.60 K**			
CSID	21106179	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	70.0138	**H bond donors**	0	**ACD/LogP**	0.48
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	FC(F)F				
STD InChIKey	XPDWGBQVDMORPB-UHFFFAOYAM				

Melting Points

mp °C	source
-160.00	Oxford University MSDS
-155.10	PHYSPROP

fluoromethane CH3F[28, 49, 61, 64]

Compound Data

Melting point	**-142.32 °C**	**130.83 K**			
CSID	11148	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	34.0329	**H bond donors**	0	**ACD/LogP**	0.51
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.67 g/cm^3
SMILES	FC				
STD InChIKey	NBVXSUQYWXRMNV-UHFFFAOYAF				

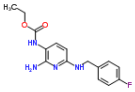
Melting Points

mp °C	source
-143.30	CRC Handbook of Chemistry and Physics
-141.85	KDB
-141.80	PHYSPROP
	Values not used in calculating the average melting point
-115.00	Oxford University MSDS[1]

1. clearly out of range and analog trend JCB

flupirtine C15H17FN4O2[9, 48, 64]

Compound Data



Melting point	**114.50 °C**	**387.65 K**			
CSID	48119	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	304.3195	**H bond donors**	4	**ACD/LogP**	1.46
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.35 g/cm^3
SMILES	Fc1ccc(cc1)CNc2nc(N)c(NC(=O)OCC)cc2				
STD InChIKey	JUUFBMODXQKSTD-UHFFFAOYAW				

Melting Points

mp °C	source
114.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
114.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
115.50	PHYSPROP

formamide CH3NO[3, 61, 64]

Compound Data

Melting point	**2.18 °C**	**275.33 K**			
CSID	693	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	45.0406	**H bond donors**	2	**ACD/LogP**	-1.51
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.98 g/cm^3
SMILES	O=CN				
STD InChIKey	ZHNUHDYFZUAESO-UHFFFAOYAQ				

Melting Points

mp °C	source
2.00	Alfa Aesar
2.00	Oxford University MSDS
2.55	PHYSPROP

formic acid CH2O2[3, 35, 51, 64]

Compound Data

Melting point	**8.23 °C**	**281.38 K**			
CSID	278	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	46.0254	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	C(=O)O				
STD InChIKey	BDAGIHXWWSANSR-UHFFFAOYAT				

Melting Points

mp °C	source
8.00	Alfa Aesar
8.30	EPISuite-ChemSpider
8.32	Kohler F; Atrops H; Kalali H; Libermann E; Wilhelm E; Ratkov...
8.30	PHYSPROP

formic acid hydrazide CH4N2O[3, 64]

Compound Data

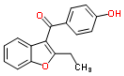
Melting point	**56.00 °C**	**329.15 K**			
CSID	11728	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	60.0553	**H bond donors**	3	**ACD/LogP**	-2.05
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	O=CNN				
STD InChIKey	XZBIXDPGRMLSTC-UHFFFAOYAQ				

Melting Points

mp °C	source
57.00	Alfa Aesar
55.00	PHYSPROP

fragivil C17H14O3[9, 48, 64]

Compound Data



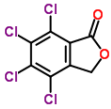
Melting point	**124.10 °C**	**397.25 K**			
CSID	224468	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	266.2913	**H bond donors**	1	**ACD/LogP**	4.31
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.23 g/cm^3
SMILES	O=C(c1c2ccccc2oc1CC)c3ccc(O)cc3				
STD InChIKey	RFRXIWQYSOIBDI-UHFFFAOYAV				

Melting Points

mp °C	source
124.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
124.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
124.30	PHYSPROP

fthalide C8H2Cl4O2[48, 64]

Compound Data



Melting point	**208.75 °C**	**481.90 K**			
CSID	31144	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	271.9123	**H bond donors**	0	**ACD/LogP**	2.73
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.77 g/cm^3
SMILES	O=C1OCc2c1c(Cl)c(Cl)c(Cl)c2Cl				
STD InChIKey	NMWKWBPNKPGATC-UHFFFAOYAH				

Melting Points

mp °C	source
208.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
209.50	PHYSPROP

furan C4H4O[3, 61, 64]

Compound Data

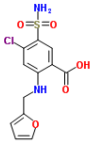
Melting point	**-85.40 °C**	**187.75 K**			
CSID	7738	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	68.074	**H bond donors**	0	**ACD/LogP**	1.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.94 g/cm^3
SMILES	c1ccoc1				
STD InChIKey	YLQBMQCUIZJEEH-UHFFFAOYAC				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-85.60	Oxford University MSDS
-85.60	PHYSPROP

furosemide C12H11ClN2O5S[16, 26, 29, 32, 33, 35, 44, 64, 71, 72, 72]

Compound Data



Melting point	**205.75 °C**	**478.90 K**			
CSID	3322	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	330.7441	**H bond donors**	4	**ACD/LogP**	3.10
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.61 g/cm^3
SMILES	O=S(=O)(N)c1c(Cl)cc(c(C(=O)O)c1)NCc2occc2				
STD InChIKey	ZZUFCTLCJUWOSV-UHFFFAOYAU				

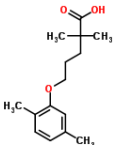
Melting Points

mp °C	source
206.00	CasLab
208.00	Crystal Growth and Design
206.00	DrugBank
204.00	ElephantCare
204.50	Shin S; Kim J. International Journal of Pharmaceutics 251(1-...
206.00	Sigma-Aldrich
	Values not used in calculating the average melting point
220.00	ConvaChem[1]
295.00	EPISuite-ChemSpider[2]
295.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...[3]
295.00	PHYSPROP[4]
220.00	Sigma-Aldrich[5]

1. only one value here while many cluster around 206C JCB
2. only one value here while many cluster around 206C JCB
3. only one value here while many cluster around 206C JCB
4. only one value here while many cluster around 206C JCB
5. only one value here while many cluster around 206C JCB

gemfibrozil C15H22O3[9, 48, 64]

Compound Data



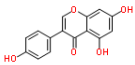
Melting point	**61.33 °C**	**334.48 K**			
CSID	3345	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	250.3334	**H bond donors**	1	**ACD/LogP**	4.39
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.04 g/cm^3
SMILES	O=C(O)C(C)(C)CCCOc1cc(ccc1C)C				
STD InChIKey	HEMJJKBWTPKOJG-UHFFFAOYAS				

Melting Points

mp °C	source
61.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
61.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
62.00	PHYSPROP

genistein C15H10O5[3, 32]

Compound Data



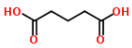
Melting point	**300.75 °C**	**573.90 K**			
CSID	4444448	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	270.2369	**H bond donors**	3	**ACD/LogP**	2.96
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.55 g/cm^3
SMILES	Oc1ccc(cc1)C\3=C\Oc2cc(O)cc(O)c2C/3=O				
STD InChIKey	TZBJGXHYKVUXJN-UHFFFAOYAH				

Melting Points

mp °C	source
300.00	Alfa Aesar
301.50	DrugBank

glutaric acid C5H8O4[3, 61, 64]

Compound Data



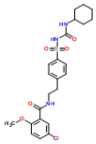
Melting point	**97.10 °C**	**370.25 K**			
CSID	723	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	132.1146	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.32 g/cm^3
SMILES	C(CC(=O)O)CC(=O)O				
STD InChIKey	JFCQEDHGNNZCLN-UHFFFAOYAU				

Melting Points

mp °C	source
97.00	Alfa Aesar
96.50	Oxford University MSDS
97.80	PHYSPROP

glyburide C23H28ClN3O5S[3, 9, 32, 64]

Compound Data



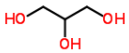
Melting point	**170.12 °C**	**443.27 K**			
CSID	3368	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	494.0035	**H bond donors**	3	**ACD/LogP**	3.75
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.36 g/cm^3
SMILES	O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)CCNC(=O)c3cc(Cl)ccc3OC				
STD InChIKey	ZNNLBTZKUZBEKO-UHFFFAOYAK				

Melting Points

mp °C	source
173.00	Alfa Aesar
169.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
169.50	DrugBank
169.00	PHYSPROP

glycerol C3H8O3[3, 61, 64]

Compound Data



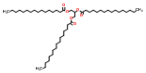
Melting point	**18.00 °C**	**291.15 K**			
CSID	733	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	92.0938	**H bond donors**	3	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.30 g/cm^3
SMILES	C(C(CO)O)O				
STD InChIKey	PEDCQBHIVMGVHV-UHFFFAOYAF				

Melting Points

mp °C	source
18.00	Alfa Aesar
17.80	Oxford University MSDS
18.20	PHYSPROP

glycerol tripalmitate C51H98O6[3, 64]

Compound Data

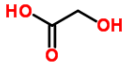


Melting point	**64.25 °C**	**337.40 K**			
CSID	10674	**H bond acceptors**	6	**Rule of 5 violations**	2
Molecular weight	807.3202	**H bond donors**	0	**ACD/LogP**	22.08
Phase 25 °C	solid	**Rotatable bonds**	50	**Predicted density**	0.92 g/cm^3
SMILES	O=C(OCC(OC(=O)CCCCCCCCCCCCCCC)COC(=O)CCCCCCCCCCCCCCC)CCCCCCCCCCCCCCC				
STD InChIKey	PVNIQBQSYATKKL-UHFFFAOYAV				

Melting Points

mp °C	source
62.00	Alfa Aesar
66.50	PHYSPROP

glycolic acid C2H4O3[3, 61, 64]



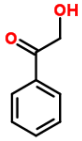
Compound Data

Melting point	**78.83 °C**	**351.98 K**			
CSID	737	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	76.0514	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.42 g/cm^3
SMILES	C(C(=O)O)O				
STD InChIKey	AEMRFAOFKBGASW-UHFFFAOYAR				

Melting Points

mp °C	source
77.00	Alfa Aesar
80.00	Oxford University MSDS
79.50	PHYSPROP

glycolophenone C8H8O2[2, 3, 17, 59, 64]



Compound Data

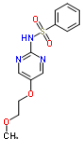
Melting point	**5.17 °C**	**278.32 K**			
CSID	61765	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	1	**ACD/LogP**	0.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	O=C(c1ccccc1)CO				
STD InChIKey	ZWVHTXAYIKBMEE-UHFFFAOYAZ				

Melting Points

mp °C	source
6.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
4.50	Alfa Aesar
5.00	ChemBlink
	Values not used in calculating the average melting point
28.00	NIST Web Book[1]
90.00	PHYSPROP[2]

1. clearly out of range JCB
2. clearly out of range JCB

glymidine C13H15N3O4S[9, 64]



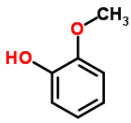
Compound Data

Melting point	**152.50 °C**	**425.65 K**			
CSID	9190	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	309.3409	**H bond donors**	1	**ACD/LogP**	1.05
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.35 g/cm^3
SMILES	O=S(=O)(Nc1ncc(OCCOC)cn1)c2ccccc2				
STD InChIKey	QFWPJPIVLCBXFJ-UHFFFAOYAT				

Melting Points

mp °C	source
152.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
153.00	PHYSPROP

guaiacol C7H8O2[2, 3, 61, 64]



Compound Data

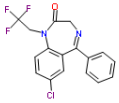
Melting point	**29.50 °C**	**302.65 K**			
CSID	447	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	1	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.11 g/cm^3
SMILES	COc1ccccc1O				
STD InChIKey	LHGVFZTZFXWLCP-UHFFFAOYAI				

Melting Points

mp °C	source
28.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
30.00	Alfa Aesar
28.00	Oxford University MSDS
32.00	PHYSPROP

halazepam C17H12ClF3N2O[9, 48, 64]

Compound Data



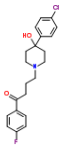
Melting point	**164.33 °C**	**437.48 K**			
CSID	29343	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	352.7382	**H bond donors**	0	**ACD/LogP**	4.22
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.37 g/cm^3
SMILES	FC(F)(F)CN1C(=O)C/N=C(\c2cc(Cl)ccc12)c3ccccc3				
STD InChIKey	WYCLKVQLVUQKNZ-UHFFFAOYAZ				

Melting Points

mp °C	source
164.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
164.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
165.00	PHYSPROP

haloperidol C21H23ClFNO2[9, 32, 35, 44, 48, 64]

Compound Data



Melting point	**149.87 °C**	**423.02 K**			
CSID	3438	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	375.8642	**H bond donors**	1	**ACD/LogP**	3.76
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.24 g/cm^3
SMILES	c1cc(ccc1C(=O)CCCN2CCC(CC2)(c3ccc(cc3)Cl)O)F				
STD InChIKey	LNEPOXFFQSENCJ-UHFFFAOYAL				

Melting Points

mp °C	source
148.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
151.50	DrugBank
151.50	EPISuite-ChemSpider
148.70	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
148.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
151.50	PHYSPROP

henicosane C21H44[3, 61, 64]

Compound Data

Melting point	**40.17 °C**	**313.32 K**			
CSID	11897	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	296.5741	**H bond donors**	0	**ACD/LogP**	11.91
Phase 25 °C	solid	**Rotatable bonds**	18	**Predicted density**	0.79 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCC)CC				
STD InChIKey	FNAZRRHPUDJQCJ-UHFFFAOYAL				

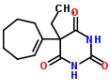
Melting Points

mp °C	source
41.00	Alfa Aesar
39.00	Oxford University MSDS
40.50	PHYSPROP

heptabarbital C13H18N2O3[9, 32, 44, 48, 64]

Compound Data

Melting point	**174.20 °C**	**447.35 K**



CSID	10081	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	250.2936	**H bond donors**	2	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(/C2=C/CCCCC2)CC				
STD InChIKey	PAZQYDJGLKSCSI-UHFFFAOYAO				

Melting Points

mp °C	source
174.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
174.00	DrugBank
175.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
174.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
174.00	PHYSPROP

heptacosane C27H56[3, 64]

Compound Data

Melting point	**59.25 °C**	**332.40 K**			
CSID	11146	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	380.7335	**H bond donors**	0	**ACD/LogP**	15.10
Phase 25 °C	solid	**Rotatable bonds**	24	**Predicted density**	0.80 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCC)CCCCC				
STD InChIKey	BJQWYEJQWHSSCJ-UHFFFAOYAK				

Melting Points

mp °C	source
59.00	Alfa Aesar
59.50	PHYSPROP

heptadecane C17H36[3, 4, 61, 64]

Compound Data

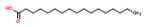
Melting point	**21.75 °C**	**294.90 K**			
CSID	11892	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	240.4677	**H bond donors**	0	**ACD/LogP**	9.79
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	0.78 g/cm^3
SMILES	CCCCCCCCCCCCCCCCC				
STD InChIKey	NDJKXXJCMXVBJW-UHFFFAOYAV				

Melting Points

mp °C	source
22.00	Alfa Aesar
22.00	American Petroleum Institute. Research Project 44; Selected ...
21.00	Oxford University MSDS
22.00	PHYSPROP

heptadecanoic acid C17H34O2[3, 61, 64]

Compound Data



Melting point	**60.77 °C**	**333.92 K**			
CSID	10033	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	270.4507	**H bond donors**	1	**ACD/LogP**	7.68
Phase 25 °C	solid	**Rotatable bonds**	15	**Predicted density**	0.89 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCCCC				
STD InChIKey	KEMQGTRYUADPNZ-UHFFFAOYAT				

Melting Points

mp °C	source
61.00	Alfa Aesar
60.00	Oxford University MSDS
61.30	PHYSPROP

heptafluorobutyric acid C4HF7O2[3, 64]

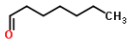
Compound Data

Melting point	**-17.75 °C**	**255.40 K**			
CSID	9394	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	214.0384	**H bond donors**	1	**ACD/LogP**	3.93
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.68 g/cm^3
SMILES	FC(F)(C(F)(F)C(=O)O)C(F)(F)F				
STD InChIKey	YPJUNDFVDDCYIH-UHFFFAOYAI				

Melting Points

mp °C	source
-18.00	Alfa Aesar
-17.50	PHYSPROP

heptanal C7H14O[3, 4, 61, 64]



Compound Data

Melting point	**-43.08 °C**	**230.07 K**			
CSID	7838	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	114.1855	**H bond donors**	0	**ACD/LogP**	2.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.81 g/cm^3
SMILES	O=CCCCCCC				
STD InChIKey	FXHGMKSSBGDXIY-UHFFFAOYAJ				

Melting Points

mp °C	source
-43.00	Alfa Aesar
-43.00	American Petroleum Institute. Research Project 44; Selected ...
-43.00	Oxford University MSDS
-43.30	PHYSPROP

heptane C7H16[3, 4, 59, 61, 64]

Compound Data

Melting point	**-90.84 °C**	**182.31 K**			
CSID	8560	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	100.2019	**H bond donors**	0	**ACD/LogP**	4.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.69 g/cm^3
SMILES	CCCCCCC				
STD InChIKey	IMNFDUFMRHMDMM-UHFFFAOYAU				

Melting Points

mp °C	source
-91.00	Alfa Aesar
-91.00	American Petroleum Institute. Research Project 44; Selected ...
-90.59	NIST Web Book
-91.00	Oxford University MSDS
-90.60	PHYSPROP

heptanenitrile C7H13N[3, 31]

Compound Data

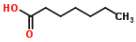
Melting point	**-63.50 °C**	**209.65 K**			
CSID	11866	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	111.1848	**H bond donors**	0	**ACD/LogP**	2.21
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.81 g/cm^3
SMILES	N#CCCCCCC				
STD InChIKey	SDAXRHHPNYTELL-UHFFFAOYAT				

Melting Points

mp °C	source

-64.00	Alfa Aesar
-63.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...

heptanoic acid C7H14O2[3, 4, 61, 64]



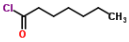
Compound Data

Melting point	**-7.62 °C**	**265.52 K**			
CSID	7803	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1849	**H bond donors**	1	**ACD/LogP**	2.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.94 g/cm^3
SMILES	O=C(O)CCCCCC				
STD InChIKey	MNWFXJYAOYHMED-UHFFFAOYAP				

Melting Points

mp °C	source
-8.00	Alfa Aesar
-6.00	American Petroleum Institute. Research Project 44; Selected ...
-9.00	Oxford University MSDS
-7.50	PHYSPROP

heptanoyl chloride C7H13ClO[3, 64]



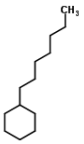
Compound Data

Melting point	**-83.90 °C**	**189.25 K**			
CSID	16383	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	148.6305	**H bond donors**	0	**ACD/LogP**	3.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.97 g/cm^3
SMILES	ClC(=O)CCCCCC				
STD InChIKey	UCVODTZQZHMTPN-UHFFFAOYAG				

Melting Points

mp °C	source
-84.00	Alfa Aesar
-83.80	PHYSPROP

heptylcyclohexane C13H26[4, 64]



Compound Data

Melting point	**-30.50 °C**	**242.65 K**			
CSID	20521	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	182.3455	**H bond donors**	0	**ACD/LogP**	7.07
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.80 g/cm^3
SMILES	C(CCC1CCCCC1)CCCC				
STD InChIKey	MSTLSCNJAHAQNU-UHFFFAOYAB				

Melting Points

mp °C	source
-31.00	American Petroleum Institute. Research Project 44; Selected ...
-30.00	PHYSPROP

hexabromobenzene C6Br6[61, 64]

Compound Data

Melting point	**326.50 °C**	**599.65 K**			
CSID	6639	**H bond acceptors**	0	**Rule of 5 violations**	2
Molecular weight	551.4882	**H bond donors**	0	**ACD/LogP**	5.85
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.96 g/cm^3
SMILES	Brc1c(Br)c(Br)c(Br)c(Br)c1Br				
STD InChIKey	CAYGQBVSOZLICD-UHFFFAOYAA				

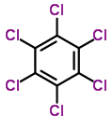
Melting Points

mp °C	source

327.00	Oxford University MSDS
326.00	PHYSPROP

hexachlorobenzene C6Cl6[44, 61, 64, 70, 70]

Compound Data



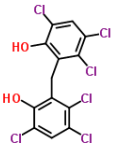
Melting point	**230.16 °C**	**503.31 K**			
CSID	8067	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	284.7822	**H bond donors**	0	**ACD/LogP**	5.75
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.77 g/cm^3
SMILES	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl				
STD InChIKey	CKAPSXZOOQJIBF-UHFFFAOYAV				

Melting Points

mp °C	source
231.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
228.00	Oxford University MSDS
231.80	PHYSPROP
230.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
230.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

hexachlorophene C13H6Cl6O2[61, 64]

Compound Data



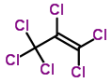
Melting point	**165.25 °C**	**438.40 K**			
CSID	3472	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	406.9035	**H bond donors**	2	**ACD/LogP**	7.20
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.71 g/cm^3
SMILES	Clc1c(c(O)c(Cl)cc1Cl)Cc2c(O)c(Cl)cc(Cl)c2Cl				
STD InChIKey	ACGUYXCXAPNIKK-UHFFFAOYAL				

Melting Points

mp °C	source
164.00	Oxford University MSDS
166.50	PHYSPROP

hexachloropropene C3Cl6[3, 64]

Compound Data



Melting point	**-72.95 °C**	**200.20 K**			
CSID	15113	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	248.7501	**H bond donors**	0	**ACD/LogP**	6.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.78 g/cm^3
SMILES	Cl/C(Cl)=C(/Cl)C(Cl)(Cl)Cl				
STD InChIKey	VFDYKPARTDCDCU-UHFFFAOYAH				

Melting Points

mp °C	source
-73.00	Alfa Aesar
-72.90	PHYSPROP

hexacosane C26H54[3, 64]

Compound Data

Melting point	**56.70 °C**	**329.85 K**			
CSID	11901	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	366.707	**H bond donors**	0	**ACD/LogP**	14.57
Phase 25 °C	solid	**Rotatable bonds**	23	**Predicted density**	0.80 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCC)CCCCC				
STD InChIKey	HMSWAIKSFDFLKN-UHFFFAOYAN				

Melting Points

mp °C	source
57.00	Alfa Aesar
56.40	PHYSPROP

hexadecane C16H34[3, 4, 61, 64]

Compound Data

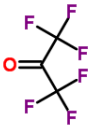
Melting point	**18.02 °C**	**291.17 K**			
CSID	10540	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	226.4412	**H bond donors**	0	**ACD/LogP**	8.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	13	**Predicted density**	0.77 g/cm^3
SMILES	CCCCCCCCCCCCCCCC				
STD InChIKey	DCAYPVUWAIABOU-UHFFFAOYAR				

Melting Points

mp °C	source
18.00	Alfa Aesar
18.00	American Petroleum Institute. Research Project 44; Selected ...
18.00	Oxford University MSDS
18.10	PHYSPROP

hexafluoroacetone C3F6O[61, 64, 64]

Compound Data



Melting point	**-127.00 °C**	**146.15 K**			
CSID	13846015	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	166.0219	**H bond donors**	0	**ACD/LogP**	1.89
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.54 g/cm^3
SMILES	FC(F)(F)C(=O)C(F)(F)F				
STD InChIKey	VBZWSGALLODQNC-UHFFFAOYAI				

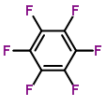
Melting Points

mp °C	source
-129.00	Oxford University MSDS
-125.00	PHYSPROP
	Values not used in calculating the average melting point
19.50	PHYSPROP[1]

1. hydrate JCB

hexafluorobenzene C6F6[3, 61, 64]

Compound Data



Melting point	**4.73 °C**	**277.88 K**			
CSID	13836549	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	186.0546	**H bond donors**	0	**ACD/LogP**	2.42
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.62 g/cm^3
SMILES	Fc1c(F)c(F)c(F)c(F)c1F				
STD InChIKey	ZQBFAOFFOQMSGJ-UHFFFAOYAJ				

Melting Points

mp °C	source
5.00	Alfa Aesar
3.90	Oxford University MSDS
5.30	PHYSPROP

hexafluoroethane C2F6[61, 64]

Compound Data

Melting point	**-100.35 °C**	**172.80 K**			
CSID	6191	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	138.0118	**H bond donors**	0	**ACD/LogP**	2.00

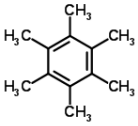
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.46 g/cm
SMILES	FC(F)(F)C(F)(F)F				
STD InChIKey	WMIYKQLTONQJES-UHFFFAOYAP				

Melting Points

mp °C	source
-100.00	Oxford University MSDS
-100.70	PHYSPROP

hexamethylbenzene C12H18[2, 3, 64, 70]

Compound Data



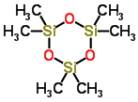
Melting point	**164.88 °C**	**438.02 K**			
CSID	6642	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	162.2713	**H bond donors**	0	**ACD/LogP**	4.98
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1(c(c(c(c(c1C)C)C)C)C)C				
STD InChIKey	YUWFEBAXEOLKSG-UHFFFAOYAF				

Melting Points

mp °C	source
164.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
165.00	Alfa Aesar
166.50	PHYSPROP
164.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

hexamethylcyclotrisiloxane C6H18O3Si3[3, 61, 64]

Compound Data



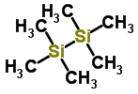
Melting point	**63.17 °C**	**336.32 K**			
CSID	10452	**H bond acceptors**	3	**Rule of 5 violations**	NA
Molecular weight	222.4618	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.94 g/cm^3
SMILES	O1[Si](O[Si](O[Si]1(C)C)(C)C)(C)C				
STD InChIKey	HTDJPCNNEPUOOQ-UHFFFAOYAR				

Melting Points

mp °C	source
65.00	Alfa Aesar
60.00	Oxford University MSDS
64.50	PHYSPROP

hexamethyldisilane C6H18Si2[3, 64]

Compound Data

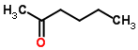


Melting point	**12.75 °C**	**285.90 K**			
CSID	66675	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	146.3781	**H bond donors**	0	**ACD/LogP**	2.50
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.73 g/cm^3
SMILES	C[Si](C)(C)[Si](C)(C)C				
STD InChIKey	NEXSMEBSBIABKL-UHFFFAOYAV				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.50	PHYSPROP

hexan-2-one C6H12O[3, 4, 61, 64]



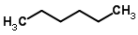
Compound Data

Melting point	**-56.12 °C**	**217.02 K**			
CSID	11095	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	100.1589	**H bond donors**	0	**ACD/LogP**	1.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.80 g/cm^3
SMILES	O=C(C)CCCC				
STD InChIKey	QQZOPKMRPOGIEB-UHFFFAOYAQ				

Melting Points

mp °C	source
-56.00	Alfa Aesar
-56.00	American Petroleum Institute. Research Project 44; Selected ...
-57.00	Oxford University MSDS
-55.50	PHYSPROP

hexane C6H14[3, 4, 32, 59, 61, 64]



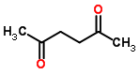
Compound Data

Melting point	**-95.12 °C**	**178.02 K**			
CSID	7767	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	86.1754	**H bond donors**	0	**ACD/LogP**	3.76
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.68 g/cm^3
SMILES	CCCCCC				
STD InChIKey	VLKZOEOYAKHREP-UHFFFAOYAD				

Melting Points

mp °C	source
-95.00	Alfa Aesar
-95.00	American Petroleum Institute. Research Project 44; Selected ...
-95.30	DrugBank
-95.15	NIST Web Book
-95.00	Oxford University MSDS
-95.30	PHYSPROP

hexane-2,5-dione C6H10O2[2, 3, 61, 64]



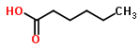
Compound Data

Melting point	**-6.12 °C**	**267.02 K**			
CSID	7744	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.1424	**H bond donors**	0	**ACD/LogP**	-0.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.94 g/cm^3
SMILES	O=C(C)CCC(=O)C				
STD InChIKey	OJVAMHKKJGICOG-UHFFFAOYAH				

Melting Points

mp °C	source
-6.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-6.00	Alfa Aesar
-7.00	Oxford University MSDS
-5.50	PHYSPROP

hexanoic acid C6H12O2[3, 4, 10, 35, 61, 64]



Compound Data

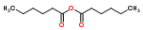
Melting point	**-2.98 °C**	**270.17 K**			
CSID	8552	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	1	**ACD/LogP**	1.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.95 g/cm^3
SMILES	CCCCCC(=O)O				
STD InChIKey	FUZZWVXGSFPDMH-UHFFFAOYAY				

Melting Points

mp °C	source
-4.00	Alfa Aesar
-3.00	American Petroleum Institute. Research Project 44; Selected ...
-1.90	Bica K.; Shamshina J.; Hough WL.; MacFarlane DR.; Rogers RD....
-3.00	EPISuite-ChemSpider
-3.00	Oxford University MSDS
-3.00	PHYSPROP

hexanoic anhydride C12H22O3[3, 64]

Compound Data



Melting point	**-40.50 °C**	**232.65 K**			
CSID	67479	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.3013	**H bond donors**	0	**ACD/LogP**	3.77
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	0.94 g/cm^3
SMILES	O=C(OC(=O)CCCCC)CCCCC				
STD InChIKey	PKHMTIRCAFTBDS-UHFFFAOYAZ				

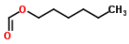
Melting Points

mp °C	source
-40.00	Alfa Aesar
-41.00	PHYSPROP

hexatriacontane C36H74[3, 64]

Compound Data

Melting point	**76.25 °C**	**349.40 K**			
CSID	11906	**H bond acceptors**	0	**Rule of 5 violations**	2
Molecular weight	506.9728	**H bond donors**	0	**ACD/LogP**	19.88
Phase 25 °C	solid	**Rotatable bonds**	33	**Predicted density**	0.81 g/cm^3
SMILES	C(CCCC

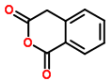


SMILES	O=COCCCCCC
STD InChIKey	OUGPMNMLWKSBRI-UHFFFAOYAA

Melting Points

mp °C	source
-63.00	Alfa Aesar
-62.60	PHYSPROP

homophthalic anhydride C9H6O3[3, 48]



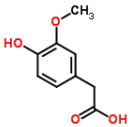
Compound Data

Melting point	**142.50 °C**	**415.65 K**			
CSID	12274	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	162.1421	**H bond donors**	0	**ACD/LogP**	0.41
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.35 g/cm^3
SMILES	O=C1OC(=O)Cc2ccccc12				
STD InChIKey	AKHSBAVQPIRVAG-UHFFFAOYAF				

Melting Points

mp °C	source
142.00	Alfa Aesar
143.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

homovanillic acid C9H10O4[3, 64]



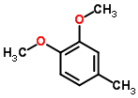
Compound Data

Melting point	**143.25 °C**	**416.40 K**			
CSID	1675	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.1733	**H bond donors**	2	**ACD/LogP**	0.47
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.31 g/cm^3
SMILES	O=C(O)Cc1cc(OC)c(O)cc1				
STD InChIKey	QRMZSPFSDQBLIX-UHFFFAOYAZ				

Melting Points

mp °C	source
143.00	Alfa Aesar
143.50	PHYSPROP

homoveratrol C9H12O2[3, 64]



Compound Data

Melting point	**25.50 °C**	**298.65 K**			
CSID	61434	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	152.1904	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	Cc1ccc(c(c1)OC)OC				
STD InChIKey	GYPMBQZAVBFUIZ-UHFFFAOYAG				

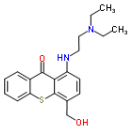
Melting Points

mp °C	source
27.00	Alfa Aesar
24.00	PHYSPROP

hycanthone C20H24N2O2S[9, 48, 64]

Compound Data

Melting point	**101.30 °C**	**374.45 K**			
CSID	3508	**H bond acceptors**	4	**Rule of 5 violations**	0



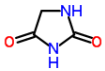
Molecular weight	356.4818	**H bond donors**	2	**ACD/LogP**	3.09
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.25 g/cm^3
SMILES	O=C1c3ccccc3Sc2c1c(ccc2CO)NCCN(CC)CC				
STD InChIKey	MFZWMTSUNYWVBU-UHFFFAOYAX				

Melting Points

mp °C	source
101.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
101.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
101.90	PHYSPROP

hydantoin C3H4N2O2[3, 48, 64]

Compound Data



Melting point	**221.00 °C**	**494.15 K**			
CSID	9612	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	100.0761	**H bond donors**	2	**ACD/LogP**	-1.69
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.36 g/cm^3
SMILES	O=C1NC(=O)NC1				
STD InChIKey	WJRBRSLFGCUECM-UHFFFAOYAD				

Melting Points

mp °C	source
222.00	Alfa Aesar
221.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
220.00	PHYSPROP

hydroflumethiazide C8H8F3N3O4S2[9, 32, 44, 64]

Compound Data

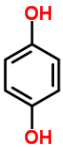
Melting point	**271.88 °C**	**545.02 K**			
CSID	3521	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	331.292	**H bond donors**	4	**ACD/LogP**	0.36
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.68 g/cm^3
SMILES	FC(F)(F)c2c(cc1c(NCNS1(=O)=O)c2)S(=O)(=O)N				
STD InChIKey	DMDGGSIALPNSEE-UHFFFAOYAE				

Melting Points

mp °C	source
272.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
272.50	DrugBank
272.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
270.50	PHYSPROP

hydroquinone C6H6O2[2, 3, 35, 64]

Compound Data



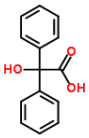
Melting point	**172.20 °C**	**445.35 K**			
CSID	764	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	110.1106	**H bond donors**	2	**ACD/LogP**	0.62
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	c1cc(ccc1O)O				
STD InChIKey	QIGBRXMKCJKVMJ-UHFFFAOYAX				

Melting Points

mp °C	source
175.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
171.00	Alfa Aesar
172.30	EPISuite-ChemSpider
170.50	PHYSPROP

hydroxydiphenylacetic acid $C_{14}H_{12}O_3$[3, 35, 48, 59, 59, 61, 64]

Compound Data



Melting point	**150.37 °C**	**423.52 K**			
CSID	6220	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	228.2433	**H bond donors**	2	**ACD/LogP**	3.03
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.28 g/cm^3
SMILES	O=C(O)C(O)(c1ccccc1)c2ccccc2				
STD InChIKey	UKXSKSHDVLQNKG-UHFFFAOYAV				

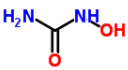
Melting Points

mp °C	source
150.00	Alfa Aesar
151.00	EPISuite-ChemSpider
148.85	NIST Web Book
149.85	NIST Web Book
151.50	Oxford University MSDS
151.00	PHYSPROP
	Values not used in calculating the average melting point
230.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...[1]

1. value clearly out of range JCB

hydroxyurea $CH_4N_2O_2$[32, 64]

Compound Data



Melting point	**142.50 °C**	**415.65 K**			
CSID	3530	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	76.0547	**H bond donors**	4	**ACD/LogP**	-1.80
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.46 g/cm^3
SMILES	O=C(N)NO				
STD InChIKey	VSNHCAURESNICA-UHFFFAOYAY				

Melting Points

mp °C	source
144.00	DrugBank
141.00	PHYSPROP

icosane $C_{20}H_{42}$[3, 4, 61, 64]

Compound Data

Melting point	**36.62 °C**	**309.77 K**			
CSID	7929	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	282.5475	**H bond donors**	0	**ACD/LogP**	11.38
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.79 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCC)CC				
STD InChIKey	CBFCDTFDPHXCNY-UHFFFAOYAJ				

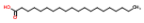
Melting Points

mp °C	source
37.00	Alfa Aesar
36.00	American Petroleum Institute. Research Project 44; Selected ...
36.70	Oxford University MSDS
36.80	PHYSPROP

icosanoic acid $C_{20}H_{40}O_2$[3, 61, 64]

Compound Data

Melting point	**75.13 °C**	**348.28 K**			
CSID	10035	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	312.5304	**H bond donors**	1	**ACD/LogP**	9.28
Phase 25 °C	solid	**Rotatable bonds**	18	**Predicted density**	0.88 g/cm^3



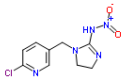
SMILES	O=C(O)CCCCCCCCCCCCCCCCCCC
STD InChIKey	VKOBVWXKNCXXDE-UHFFFAOYAB

Melting Points

mp °C	source
75.00	Alfa Aesar
75.00	Oxford University MSDS
75.40	PHYSPROP

imidacloprid C9H10ClN5O2 Oxford University MSDS, 64

Compound Data



Melting point	**142.05 °C**	**415.20 K**			
CSID	77934	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	255.661	**H bond donors**	1	**ACD/LogP**	-0.43
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.59 g/cm^3
SMILES	[O-][N+](=O)NC/1=N/CCN\1Cc2cnc(Cl)cc2				
STD InChIKey	YWTYJOPNNQFBPC-UHFFFAOYAZ				

Melting Points

mp °C	source
140.10	5-dihydro-N-nitro-1H-imidazol-2-amine.html
144.00	PHYSPROP

imidazole C3H4N2 3, 61, 64

Compound Data

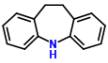
Melting point	**90.17 °C**	**363.32 K**			
CSID	773	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	68.0773	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.12 g/cm^3
SMILES	c1cnc[nH]1				
STD InChIKey	RAXXELZNTBOGNW-UHFFFAOYAS				

Melting Points

mp °C	source
90.00	Alfa Aesar
90.00	Oxford University MSDS
90.50	PHYSPROP

iminodibenzyl C14H13N 3, 64

Compound Data



Melting point	**106.75 °C**	**379.90 K**			
CSID	9886	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	195.2597	**H bond donors**	1	**ACD/LogP**	4.03
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	c1cc3c(cc1)CCc2c(cccc2)N3				
STD InChIKey	ZSMRRZONCYIFNB-UHFFFAOYAX				

Melting Points

mp °C	source
107.00	Alfa Aesar
106.50	PHYSPROP

indane C9H10 3, 64

Compound Data

Melting point	**-51.20 °C**	**221.95 K**			
CSID	9903	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	118.1757	**H bond donors**	0	**ACD/LogP**	3.21
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	c1ccc2c(c1)CCC2				
STD InChIKey	PQNFLJBBNBOBRQ-UHFFFAOYAW				

Melting Points

mp °C	source
-51.00	Alfa Aesar
-51.40	PHYSPROP

indene C9H8[3, 64]

Compound Data

Melting point	**-1.90 °C**	**271.25 K**			
CSID	6949	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	116.1598	**H bond donors**	0	**ACD/LogP**	3.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.04 g/cm^3
SMILES	c1ccc2c(c1)CC=C2				
STD InChIKey	YBYIRNPNPLQARY-UHFFFAOYAJ				

Melting Points

mp °C	source
-2.00	Alfa Aesar
-1.80	PHYSPROP

indole C8H7N[3, 61, 64]

Compound Data

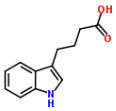
Melting point	**52.17 °C**	**325.32 K**			
CSID	776	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	117.1479	**H bond donors**	1	**ACD/LogP**	2.59
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.15 g/cm^3
SMILES	c1ccc2c(c1)cc[nH]2				
STD InChIKey	SIKJAQJRHWYJAI-UHFFFAOYAI				

Melting Points

mp °C	source
52.00	Alfa Aesar
52.00	Oxford University MSDS
52.50	PHYSPROP

indole-3-butyric acid C12H13NO2[3, 32, 64]

Compound Data



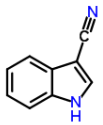
Melting point	**124.00 °C**	**397.15 K**			
CSID	8298	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	203.2371	**H bond donors**	2	**ACD/LogP**	2.34
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=C(O)CCCc2c1ccccc1nc2				
STD InChIKey	JTEDVYBZBROSJT-UHFFFAOYAT				

Melting Points

mp °C	source
123.00	Alfa Aesar
124.50	DrugBank
124.50	PHYSPROP

indole-3-carbonitrile C9H6N2[3, 64]

Compound Data



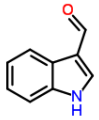
Melting point	**180.25 °C**	**453.40 K**			
CSID	200562	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	142.1573	**H bond donors**	1	**ACD/LogP**	2.32
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	N#Cc2c1ccccc1nc2				
STD InChIKey	CHIFTAQVXHNVRW-UHFFFAOYAG				

Melting Points

mp °C	source
180.00	Alfa Aesar
180.50	PHYSPROP

indole-3-carboxaldehyde C9H7NO[3, 64]

Compound Data



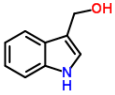
Melting point	**196.75 °C**	**469.90 K**			
CSID	9838	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	145.158	**H bond donors**	1	**ACD/LogP**	1.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.28 g/cm^3
SMILES	c1ccc2c(c1)c(c[nH]2)C=O				
STD InChIKey	OLNJUISKUQQNIM-UHFFFAOYAL				

Melting Points

mp °C	source
197.00	Alfa Aesar
196.50	PHYSPROP

indole-3-methanol C9H9NO[3, 64]

Compound Data



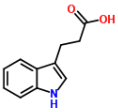
Melting point	**97.75 °C**	**370.90 K**			
CSID	3581	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	147.1739	**H bond donors**	2	**ACD/LogP**	0.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.27 g/cm^3
SMILES	OCc2c1ccccc1nc2				
STD InChIKey	IVYPNXXAYMYVSP-UHFFFAOYAO				

Melting Points

mp °C	source
98.00	Alfa Aesar
97.50	PHYSPROP

indole-3-propionic acid C11H11NO2[3, 64]

Compound Data



Melting point	**134.25 °C**	**407.40 K**			
CSID	3613	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	189.2105	**H bond donors**	2	**ACD/LogP**	1.76
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.30 g/cm^3
SMILES	O=C(O)CCc2c1ccccc1nc2				
STD InChIKey	GOLXRNDWAUTYKT-UHFFFAOYAW				

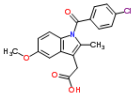
Melting Points

mp °C	source
134.00	Alfa Aesar
134.50	PHYSPROP

indomethacin C19H16ClNO4[3, 32, 44, 64]

Compound Data

Melting point	**158.95 °C**	**432.10 K**			
CSID	3584	**H bond acceptors**	5	**Rule of 5 violations**	0



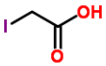
Molecular weight	357.7876	**H bond donors**	1	**ACD/LogP**	4.25
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.33 g/cm^3
SMILES	Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O				
STD InChIKey	CGIGDMFJXJATDK-UHFFFAOYAA				

Melting Points

mp °C	source
160.00	Alfa Aesar
158.00	DrugBank
159.80	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
158.00	PHYSPROP

iodoacetic acid C2H3IO2[3, 61, 64]

Compound Data



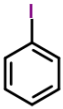
Melting point	**81.50 °C**	**354.65 K**			
CSID	5050	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	185.9485	**H bond donors**	1	**ACD/LogP**	0.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.48 g/cm^3
SMILES	C(C(=O)O)I				
STD InChIKey	JDNTWHVOXJZDSN-UHFFFAOYAA				

Melting Points

mp °C	source
81.00	Alfa Aesar
81.00	Oxford University MSDS
82.50	PHYSPROP

iodobenzene C6H5I[3, 31, 64]

Compound Data



Melting point	**-31.10 °C**	**242.05 K**			
CSID	11087	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	204.0084	**H bond donors**	0	**ACD/LogP**	3.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.83 g/cm^3
SMILES	c1ccc(cc1)I				
STD InChIKey	SNHMUERNLJLMHN-UHFFFAOYAQ				

Melting Points

mp °C	source
-31.00	Alfa Aesar
-31.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-31.30	PHYSPROP

iodoethane C2H5I[3, 31, 61, 64]

Compound Data

Melting point	**-109.53 °C**	**163.62 K**			
CSID	6100	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	155.9656	**H bond donors**	0	**ACD/LogP**	2.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.94 g/cm^3
SMILES	ICC				
STD InChIKey	HVTICUPFWKNHNG-UHFFFAOYAT				

Melting Points

mp °C	source
-108.00	Alfa Aesar
-111.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-108.00	Oxford University MSDS
-111.10	PHYSPROP

iodoform CHI3[3, 61, 64]

Compound Data

Melting point	**120.83 °C**	**393.98 K**			
CSID	6134	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	393.7321	**H bond donors**	0	**ACD/LogP**	3.51
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	3.86 g/cm^3
SMILES	IC(I)I				
STD InChIKey	OKJPEAGHQZHRQV-UHFFFAOYAY				

Melting Points

mp °C	source
122.00	Alfa Aesar
121.50	Oxford University MSDS
119.00	PHYSPROP

iodomethane CH3I[3, 31, 61, 64]

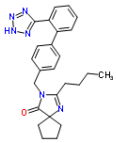
Compound Data

Melting point	**-65.85 °C**	**207.30 K**			
CSID	6088	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	141.939	**H bond donors**	0	**ACD/LogP**	1.61
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	2.22 g/cm^3
SMILES	CI				
STD InChIKey	INQOMBQAUSQDDS-UHFFFAOYAL				

Melting Points

mp °C	source
-67.00	Alfa Aesar
-66.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-64.00	Oxford University MSDS
-66.40	PHYSPROP

irbesartan C25H28N6O[9, 32, 48]



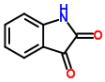
Compound Data

Melting point	**180.17 °C**	**453.32 K**			
CSID	3618	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	428.5294	**H bond donors**	1	**ACD/LogP**	4.26
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.30 g/cm^3
SMILES	O=C1N(\C(=N/C12CCCC2)CCCC)Cc5ccc(c3ccccc3c4nnnn4)cc5				
STD InChIKey	YOSHYTLCDANDAN-UHFFFAOYAO				

Melting Points

mp °C	source
180.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
180.50	DrugBank
180.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

isatin C8H5NO2[32, 61]



Compound Data

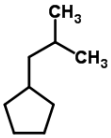
Melting point	**201.50 °C**	**474.65 K**			
CSID	6787	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	147.1308	**H bond donors**	1	**ACD/LogP**	0.56
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.37 g/cm^3
SMILES	O=C2c1ccccc1NC2=O				
STD InChIKey	JXDYKVIHCLTXOP-UHFFFAOYAS				

Melting Points

mp °C	source
203.00	DrugBank

200.00	Oxford University MSDS

iso-butylcyclopentane C9H18[4, 64]



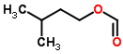
Compound Data

Melting point	**-115.10 °C**	**158.05 K**			
CSID	69826	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	126.2392	**H bond donors**	0	**ACD/LogP**	4.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.79 g/cm^3
SMILES	CC(C)CC1CCCC1				
STD InChIKey	DPUYDFJBHDYVQM-UHFFFAOYAS				

Melting Points

mp °C	source
-115.00	American Petroleum Institute. Research Project 44; Selected ...
-115.20	PHYSPROP

isoamyl formate C6H12O2[7, 64]



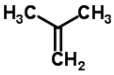
Compound Data

Melting point	**-93.25 °C**	**179.90 K**			
CSID	7761	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	0	**ACD/LogP**	1.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.88 g/cm^3
SMILES	O=COCCC(C)C				
STD InChIKey	XKYICAQFSCFURC-UHFFFAOYAX				

Melting Points

mp °C	source
-93.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
-93.50	PHYSPROP

isobutene C4H8[61, 64]



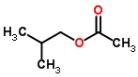
Compound Data

Melting point	**-140.20 °C**	**132.95 K**			
CSID	7957	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	56.1063	**H bond donors**	0	**ACD/LogP**	2.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.63 g/cm^3
SMILES	CC(=C)C				
STD InChIKey	VQTUBCCKSQIDNK-UHFFFAOYAW				

Melting Points

mp °C	source
-140.00	Oxford University MSDS
-140.40	PHYSPROP

isobutyl acetate C6H12O2[3, 64]



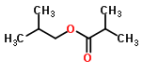
Compound Data

Melting point	**-98.90 °C**	**174.25 K**			
CSID	7747	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	0	**ACD/LogP**	1.59
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCC(C)C)C				
STD InChIKey	GJRQTCIYDGXPES-UHFFFAOYAF				

Melting Points

mp °C	source
-99.00	Alfa Aesar
-98.80	PHYSPROP

isobutyl isobutyrate $C_8H_{16}O_2$[3, 7, 64]



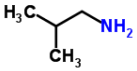
Compound Data

Melting point	**-80.57 °C**	**192.58 K**			
CSID	7073	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.2114	**H bond donors**	0	**ACD/LogP**	2.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.87 g/cm^3
SMILES	O=C(OCC(C)C)C(C)C				
STD InChIKey	RXGUIWHIADMCFC-UHFFFAOYAE				

Melting Points

mp °C	source
-81.00	Alfa Aesar
-80.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
-80.70	PHYSPROP

isobutylamine $C_4H_{11}N$[3, 31, 64]



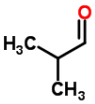
Compound Data

Melting point	**-85.67 °C**	**187.48 K**			
CSID	6310	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	73.1368	**H bond donors**	2	**ACD/LogP**	0.75
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.74 g/cm^3
SMILES	NCC(C)C				
STD InChIKey	KDSNLYIMUZNERS-UHFFFAOYAP				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-87.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-85.00	PHYSPROP

isobutyraldehyde C_4H_8O[3, 4, 61, 64]



Compound Data

Melting point	**-65.22 °C**	**207.92 K**			
CSID	6313	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	72.1057	**H bond donors**	0	**ACD/LogP**	0.76
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.78 g/cm^3
SMILES	CC(C)C=O				
STD InChIKey	AMIMRNSIRUDHCM-UHFFFAOYAE				

Melting Points

mp °C	source
-65.00	Alfa Aesar
-65.00	American Petroleum Institute. Research Project 44; Selected ...
-65.00	Oxford University MSDS
-65.90	PHYSPROP

isobutyramide C_4H_9NO[2, 3, 64]

Compound Data

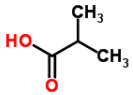
Melting point	**128.33 °C**	**401.48 K**			
CSID	61707	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	87.1204	**H bond donors**	2	**ACD/LogP**	-0.36
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.91 g/cm^3
SMILES	O=C(N)C(C)C				
STD InChIKey	WFKAJVHLWXSISD-UHFFFAOYAM				

Melting Points

mp °C	source
129.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...

128.00	Alfa Aesar
128.00	PHYSPROP

isobutyric acid C4H8O2[3, 4, 32, 64]



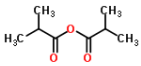
Compound Data

Melting point	**-46.25 °C**	**226.90 K**			
CSID	6341	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	1	**ACD/LogP**	0.59
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3
SMILES	O=C(O)C(C)C				
STD InChIKey	KQNPFQTWMSNSAP-UHFFFAOYAB				

Melting Points

mp °C	source
-47.00	Alfa Aesar
-46.00	American Petroleum Institute. Research Project 44; Selected ...
-46.00	DrugBank
-46.00	PHYSPROP

isobutyric anhydride C8H14O3[3, 64]



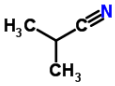
Compound Data

Melting point	**-54.75 °C**	**218.40 K**			
CSID	7069	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	158.195	**H bond donors**	0	**ACD/LogP**	1.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.98 g/cm^3
SMILES	O=C(OC(=O)C(C)C)C(C)C				
STD InChIKey	LSACYLWPPQLVSM-UHFFFAOYAZ				

Melting Points

mp °C	source
-56.00	Alfa Aesar
-53.50	PHYSPROP

isobutyronitrile C4H7N[2, 3, 61, 64]



Compound Data

Melting point	**-71.88 °C**	**201.27 K**			
CSID	6311	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	69.1051	**H bond donors**	0	**ACD/LogP**	0.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.78 g/cm^3
SMILES	N#CC(C)C				
STD InChIKey	LRDFRRGEGBBSRN-UHFFFAOYAP				

Melting Points

mp °C	source
-72.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-72.00	Alfa Aesar
-72.00	Oxford University MSDS
-71.50	PHYSPROP

isocyanuric acid triallyl ester C12H15N3O3[61, 64]

Compound Data

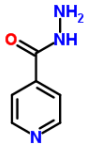
Melting point	**22.25 °C**	**295.40 K**			
CSID	13329	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	249.2658	**H bond donors**	0	**ACD/LogP**	-0.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	1.15 g/cm^3
SMILES	O=C1N(C(=O)N(C(=O)N1C\C=C)C\C=C)C\C=C				
STD InChIKey	KOMNUTZXSVSERR-UHFFFAOYAI				

Melting Points

mp °C	source
24.00	Oxford University MSDS
20.50	PHYSPROP

isoniazid C6H7N3O[3, 9, 32, 35, 44, 48, 61, 64]

Compound Data



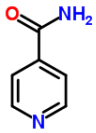
Melting point	**171.33 °C**	**444.48 K**			
CSID	3635	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	137.1393	**H bond donors**	3	**ACD/LogP**	-0.89
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	O=C(NN)c1ccncc1				
STD InChIKey	QRXWMOHMRWLFEY-UHFFFAOYAD				

Melting Points

mp °C	source
172.00	Alfa Aesar
171.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
171.40	DrugBank
171.40	EPISuite-ChemSpider
171.40	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
171.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
171.00	Oxford University MSDS
171.40	PHYSPROP

isonicotinamide C6H6N2O[3, 64]

Compound Data



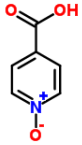
Melting point	**156.50 °C**	**429.65 K**			
CSID	14346	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	122.1246	**H bond donors**	2	**ACD/LogP**	-0.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.20 g/cm^3
SMILES	O=C(N)c1ccncc1				
STD InChIKey	VFQXVTODMYMSMJ-UHFFFAOYAE				

Melting Points

mp °C	source
157.00	Alfa Aesar
156.00	PHYSPROP

isonicotinic acid N-oxide C6H5NO3[3, 64]

Compound Data



Melting point	**270.25 °C**	**543.40 K**			
CSID	24341	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	139.1088	**H bond donors**	1	**ACD/LogP**	-1.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	[O-][n+]1ccc(C(=O)O)cc1				
STD InChIKey	QCWTWMJMLSKQCJ-UHFFFAOYAL				

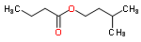
Melting Points

mp °C	source
270.00	Alfa Aesar
270.50	PHYSPROP

isopentyl butyrate C9H18O2[3, 64]

Compound Data

Melting point	**-73.10 °C**	**200.05 K**			
CSID	7507	**H bond acceptors**	2	**Rule of 5 violations**	0



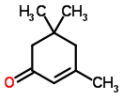
Molecular weight	158.238	**H bond donors**	0	**ACD/LogP**	3.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.87 g/cm^3
SMILES	O=C(OCCC(C)C)CCC				
STD InChIKey	PQLMXFQTAMDXIZ-UHFFFAOYAT				

Melting Points

mp °C	source
-73.00	Alfa Aesar
-73.20	PHYSPROP

isophorone C9H14O[3, 61, 64]

Compound Data



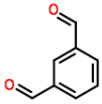
Melting point	**-8.03 °C**	**265.12 K**			
CSID	6296	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	138.2069	**H bond donors**	0	**ACD/LogP**	2.07
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.91 g/cm^3
SMILES	O=C1\C=C(/CC(C)(C)C1)C				
STD InChIKey	HJOVHMDZYOCNQW-UHFFFAOYAC				

Melting Points

mp °C	source
-8.00	Alfa Aesar
-8.00	Oxford University MSDS
-8.10	PHYSPROP

isophthalaldehyde C8H6O2[2, 47, 47, 64]

Compound Data



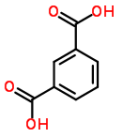
Melting point	**88.80 °C**	**361.95 K**			
CSID	32002	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	134.132	**H bond donors**	0	**ACD/LogP**	1.04
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	c1cc(cc(c1)C=O)C=O				
STD InChIKey	IZALUMVGBVKPJD-UHFFFAOYAL				

Melting Points

mp °C	source
89.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
87.85	IUCr
88.85	IUCr
89.50	PHYSPROP

isophthalic acid C8H6O4[2, 48, 64]

Compound Data



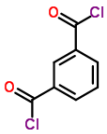
Melting point	**344.50 °C**	**617.65 K**			
CSID	8182	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	166.1308	**H bond donors**	2	**ACD/LogP**	1.66
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.45 g/cm^3
SMILES	O=C(O)c1cccc(C(=O)O)c1				
STD InChIKey	QQVIHTHCMHWDBS-UHFFFAOYAY				

Melting Points

mp °C	source
342.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
347.00	PHYSPROP
	Values not used in calculating the average melting point
68.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...[1]

1. clearly out of range JCB

isophthaloyl dichloride C8H4Cl2O2[3, 64]



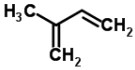
Compound Data

Melting point	**43.75 °C**	**316.90 K**			
CSID	7171	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	203.0222	**H bond donors**	0	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.43 g/cm^3
SMILES	O=C(Cl)c1cccc(C(Cl)=O)c1				
STD InChIKey	FDQSRULYDNDXQB-UHFFFAOYAQ				

Melting Points

mp °C	source
44.00	Alfa Aesar
43.50	PHYSPROP

isoprene C5H8[3, 4, 64]



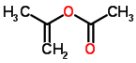
Compound Data

Melting point	**-145.97 °C**	**127.18 K**			
CSID	6309	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	68.117	**H bond donors**	0	**ACD/LogP**	2.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.67 g/cm^3
SMILES	CC(=C)C=C				
STD InChIKey	RRHGJUQNOFWUDK-UHFFFAOYAS				

Melting Points

mp °C	source
-146.00	Alfa Aesar
-146.00	American Petroleum Institute. Research Project 44; Selected ...
-145.90	PHYSPROP

isopropenyl acetate C5H8O2[3, 64]



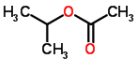
Compound Data

Melting point	**-92.95 °C**	**180.20 K**			
CSID	7628	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1158	**H bond donors**	0	**ACD/LogP**	1.28
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.91 g/cm^3
SMILES	O=C(O/C(=C)C)C				
STD InChIKey	HETCEOQFVDFGSY-UHFFFAOYAT				

Melting Points

mp °C	source
-93.00	Alfa Aesar
-92.90	PHYSPROP

isopropyl acetate C5H10O2[3, 64]



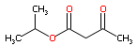
Compound Data

Melting point	**-73.20 °C**	**199.95 K**			
CSID	7627	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	0	**ACD/LogP**	1.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.89 g/cm^3
SMILES	O=C(OC(C)C)C				
STD InChIKey	JMMWKPVZQRWMSS-UHFFFAOYAA				

Melting Points

mp °C	source
-73.00	Alfa Aesar
-73.40	PHYSPROP

isopropyl acetoacetate C7H12O3[3, 64]



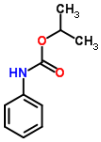
Compound Data

Melting point	**-27.15 °C**	**246.00 K**			
CSID	21171506	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	144.1684	**H bond donors**	0	**ACD/LogP**	1.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.99 g/cm^3
SMILES	CC(C)OC(=O)CC(=O)C				
STD InChIKey	GVIIRWAJDFKJMJ-UHFFFAOYAG				

Melting Points

mp °C	source
-27.00	Alfa Aesar
-27.30	PHYSPROP

isopropyl N-phenylcarbamate C10H13NO2[3, 64]



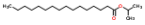
Compound Data

Melting point	**87.65 °C**	**360.80 K**			
CSID	23083	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	179.2157	**H bond donors**	1	**ACD/LogP**	2.65
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(OC(C)C)Nc1ccccc1				
STD InChIKey	VXPLXMJHHKHSOA-UHFFFAOYAY				

Melting Points

mp °C	source
88.00	Alfa Aesar
87.30	PHYSPROP

isopropyl palmitate C19H38O2[3, 64]



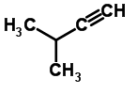
Compound Data

Melting point	**12.75 °C**	**285.90 K**			
CSID	8567	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	298.5038	**H bond donors**	0	**ACD/LogP**	8.49
Phase 25 °C	liquid/gas	**Rotatable bonds**	16	**Predicted density**	0.86 g/cm^3
SMILES	O=C(OC(C)C)CCCCCCCCCCCCCCC				
STD InChIKey	XUGNVMKQXJXZCD-UHFFFAOYAX				

Melting Points

mp °C	source
12.00	Alfa Aesar
13.50	PHYSPROP

isopropylacetylene C5H8[4, 64]



Compound Data

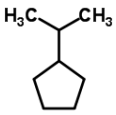
Melting point	**-89.85 °C**	**183.30 K**			
CSID	62241	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	68.117	**H bond donors**	0	**ACD/LogP**	1.88
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.71 g/cm^3
SMILES	C#CC(C)C				
STD InChIKey	USCSRAJGJYMJFZ-UHFFFAOYAZ				

Melting Points

mp °C	source
-90.00	American Petroleum Institute. Research Project 44; Selected ...
-89.70	PHYSPROP

isopropylcyclopentane C8H16[4, 64]

Compound Data



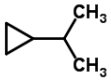
Melting point	**-111.20 °C**	**161.95 K**			
CSID	18604	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.80 g/cm^3
SMILES	CC(C)C1CCCC1				
STD InChIKey	TVSBRLGQVHJIKT-UHFFFAOYAE				

Melting Points

mp °C	source
-111.00	American Petroleum Institute. Research Project 44; Selected ...
-111.40	PHYSPROP

isopropylcyclopropane C6H12[4, 64]

Compound Data



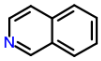
Melting point	**-112.95 °C**	**160.20 K**			
CSID	121640	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.80 g/cm^3
SMILES	CC(C)C1CC1				
STD InChIKey	HPBROFGYTXOJIO-UHFFFAOYAX				

Melting Points

mp °C	source
-113.00	American Petroleum Institute. Research Project 44; Selected ...
-112.90	PHYSPROP

isoquinoline C9H7N[3, 64]

Compound Data



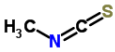
Melting point	**26.23 °C**	**299.38 K**			
CSID	8098	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.1586	**H bond donors**	0	**ACD/LogP**	2.02
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	c1ccc2ncccc2c1				
STD InChIKey	AWJUIBRHMBBTKR-UHFFFAOYAX				

Melting Points

mp °C	source
26.00	Alfa Aesar
26.47	PHYSPROP

isothiocyanatomethane C2H3NS[3, 61, 64]

Compound Data



Melting point	**34.33 °C**	**307.48 K**			
CSID	10694	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	73.1169	**H bond donors**	0	**ACD/LogP**	0.94
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.95 g/cm^3
SMILES	S=C=N/C				
STD InChIKey	LGDSHSYDSCRFAB-UHFFFAOYAS				

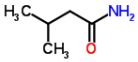
Melting Points

mp °C	source
32.00	Alfa Aesar
35.00	Oxford University MSDS
36.00	PHYSPROP

isovaleramide C5H11NO[3, 64]

Compound Data

Melting point	**136.50 °C**	**409.65 K**

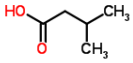


CSID	10467	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	101.1469	**H bond donors**	2	**ACD/LogP**	0.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.90 g/cm^3
SMILES	O=C(N)CC(C)C				
STD InChIKey	SANOUVWGPVYVAV-UHFFFAOYAT				

Melting Points

mp °C	source
136.00	Alfa Aesar
137.00	PHYSPROP

isovaleric acid C5H10O2[3, 4, 35, 64]



Compound Data

Melting point	**-30.40 °C**	**242.75 K**			
CSID	10001	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	1	**ACD/LogP**	1.12
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.96 g/cm^3
SMILES	O=C(O)CC(C)C				
STD InChIKey	GWYFCOCPABKNJV-UHFFFAOYAV				

Melting Points

mp °C	source
-33.00	Alfa Aesar
-30.00	American Petroleum Institute. Research Project 44; Selected ...
-29.30	EPISuite-ChemSpider
-29.30	PHYSPROP

julolidine C12H15N[3, 64]

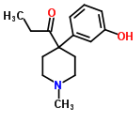
Compound Data

Melting point	**37.50 °C**	**310.65 K**			
CSID	61383	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	173.2542	**H bond donors**	0	**ACD/LogP**	3.26
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.10 g/cm^3
SMILES	c13c2c(ccc1)CCCN2CCC3				
STD InChIKey	DZFWNZJKBJOGFQ-UHFFFAOYAM				

Melting Points

mp °C	source
35.00	Alfa Aesar
40.00	PHYSPROP

ketobemidone C15H21NO2[9, 48, 64]



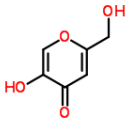
Compound Data

Melting point	**156.17 °C**	**429.32 K**			
CSID	9697	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	247.3327	**H bond donors**	1	**ACD/LogP**	1.58
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	O=C(C2(c1cccc(O)c1)CCN(C)CC2)CC				
STD InChIKey	ALFGKMXHOUSVAD-UHFFFAOYAR				

Melting Points

mp °C	source
156.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
156.50	PHYSPROP

kojic acid C6H6O4[3, 32, 64]



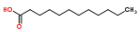
Compound Data

Melting point	**153.67 °C**	**426.82 K**			
CSID	3708	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	142.1094	**H bond donors**	2	**ACD/LogP**	-0.64
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.54 g/cm^3
SMILES	O=C1/C=C(\O/C=C1/O)CO				
STD InChIKey	BEJNERDRQOWKJM-UHFFFAOYAO				

Melting Points

mp °C	source
154.00	Alfa Aesar
153.50	DrugBank
153.50	PHYSPROP

lauric acid C12H24O2[3, 32, 61, 64]



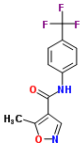
Compound Data

Melting point	**43.85 °C**	**317.00 K**			
CSID	3756	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	200.3178	**H bond donors**	1	**ACD/LogP**	5.03
Phase 25 °C	solid	**Rotatable bonds**	10	**Predicted density**	0.91 g/cm^3
SMILES	O=C(O)CCCCCCCCCCC				
STD InChIKey	POULHZVOKOAJMA-UHFFFAOYAP				

Melting Points

mp °C	source
44.00	Alfa Aesar
43.20	DrugBank
45.00	Oxford University MSDS
43.20	PHYSPROP

leflunomide C12H9F3N2O2[32, 64]



Compound Data

Melting point	**166.00 °C**	**439.15 K**			
CSID	3762	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	270.2073	**H bond donors**	1	**ACD/LogP**	1.95
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	O=C(Nc1ccc(cc1)C(F)(F)F)c2c(onc2)C				
STD InChIKey	VHOGYURTWQBHIL-UHFFFAOYAS				

Melting Points

mp °C	source
165.50	DrugBank
166.50	PHYSPROP

lepidine C10H9N[3, 64]

Compound Data

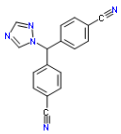
Melting point	**9.75 °C**	**282.90 K**			
CSID	13854818	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	Cc1ccnc2ccccc12				
STD InChIKey	MUDSDYNRBDKLGK-UHFFFAOYAO				

Melting Points

mp °C	source
10.00	Alfa Aesar
9.50	PHYSPROP

letrozole C17H11N5[9, 32, 48, 64]

Compound Data



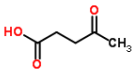
Melting point	**182.12 °C**	**455.27 K**			
CSID	3765	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	285.3027	**H bond donors**	0	**ACD/LogP**	1.92
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	N#Cc1ccc(cc1)C(c2ccc(C#N)cc2)n3ncnc3				
STD InChIKey	HPJKCIUCZWXJDR-UHFFFAOYAB				

Melting Points

mp °C	source
181.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
184.50	DrugBank
181.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
182.00	PHYSPROP

levulinic acid C5H8O3[3, 32, 64]

Compound Data



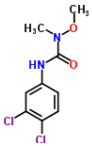
Melting point	**31.67 °C**	**304.82 K**			
CSID	11091	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	116.1152	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.13 g/cm^3
SMILES	CC(=O)CCC(=O)O				
STD InChIKey	JOOXCMJARBKPKM-UHFFFAOYAR				

Melting Points

mp °C	source
29.00	Alfa Aesar
33.00	DrugBank
33.00	PHYSPROP

linuron C9H10Cl2N2O2[44, 64]

Compound Data



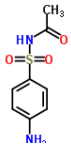
Melting point	**93.25 °C**	**366.40 K**			
CSID	9130	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	249.0939	**H bond donors**	1	**ACD/LogP**	3.20
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.41 g/cm^3
SMILES	Clc1ccc(NC(=O)N(OC)C)cc1Cl				
STD InChIKey	XKJMBINCVNINCA-UHFFFAOYAQ				

Melting Points

mp °C	source
93.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
93.00	PHYSPROP

locula C8H10N2O3S[3, 32, 44, 61, 64]

Compound Data



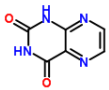
Melting point	**182.80 °C**	**455.95 K**			
CSID	5129	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	214.2416	**H bond donors**	3	**ACD/LogP**	-0.96
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.37 g/cm^3
SMILES	O=S(=O)(c1ccc(N)cc1)NC(=O)C				
STD InChIKey	SKIVFJLNDNKQPD-UHFFFAOYAW				

Melting Points

mp °C	source
183.00	Alfa Aesar
183.00	DrugBank
183.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
182.00	Oxford University MSDS

183.00	PHYSPROP

lumazine C6H4N4O2[3, 64]



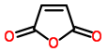
Compound Data

Melting point	**348.25 °C**	**621.40 K**			
CSID	9832	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	164.1216	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.52 g/cm^3
SMILES	c1cnc2c(n1)c(=O)[nH]c(=O)[nH]2				
STD InChIKey	UYEUUXMDVNYCAM-UHFFFAOYAF				

Melting Points

mp °C	source
348.00	Alfa Aesar
348.50	PHYSPROP

maleic anhydride C4H2O3[3, 61, 64]



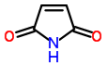
Compound Data

Melting point	**53.27 °C**	**326.42 K**			
CSID	7635	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	98.0569	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.49 g/cm^3
SMILES	C1=CC(=O)OC1=O				
STD InChIKey	FPYJFEHAWHCUMM-UHFFFAOYAP				

Melting Points

mp °C	source
54.00	Alfa Aesar
53.00	Oxford University MSDS
52.80	PHYSPROP

maleimide C4H3NO2[3, 64]



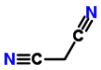
Compound Data

Melting point	**93.00 °C**	**366.15 K**			
CSID	10471	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	97.0721	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.37 g/cm^3
SMILES	C1=CC(=O)NC1=O				
STD InChIKey	PEEHTFAAVSWFBL-UHFFFAOYAL				

Melting Points

mp °C	source
92.00	Alfa Aesar
94.00	PHYSPROP

malononitrile C3H2N2[2, 3, 64]



Compound Data

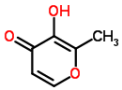
Melting point	**32.67 °C**	**305.82 K**			
CSID	13884495	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	66.0614	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.02 g/cm^3
SMILES	C(C#N)C#N				
STD InChIKey	CUONGYYJJVDODC-UHFFFAOYAD				

Melting Points

mp °C	source
34.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
32.00	Alfa Aesar

32.00	PHYSPROP

maltol C6H6O3[3, 64]



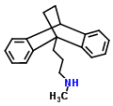
Compound Data

Melting point	**162.25 °C**	**435.40 K**			
CSID	8066	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	126.11	**H bond donors**	1	**ACD/LogP**	0.07
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.35 g/cm^3
SMILES	Cc1c(c(=O)cco1)O				
STD InChIKey	XPCTZQVDEJYUGT-UHFFFAOYAH				

Melting Points

mp °C	source
163.00	Alfa Aesar
161.50	PHYSPROP

maprotiline C20H23N[9, 48, 64]



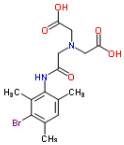
Compound Data

Melting point	**92.33 °C**	**365.48 K**			
CSID	3871	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	277.4033	**H bond donors**	1	**ACD/LogP**	4.51
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.08 g/cm^3
SMILES	c1ccc3c(c1)C4c2ccccc2C3(CC4)CCCNC				
STD InChIKey	QSLMDECMDJKHMQ-UHFFFAOYAS				

Melting Points

mp °C	source
92.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
92.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
93.00	PHYSPROP

mebrofenin C15H19BrN2O5[3, 64]



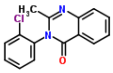
Compound Data

Melting point	**196.50 °C**	**469.65 K**			
CSID	48922	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	387.2258	**H bond donors**	3	**ACD/LogP**	3.09
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.55 g/cm^3
SMILES	Brc1c(c(c(cc1C)C)NC(=O)CN(CC(=O)O)CC(=O)O)C				
STD InChIKey	MHPZZZZLAQGTHT-UHFFFAOYAH				

Melting Points

mp °C	source
194.00	Alfa Aesar
199.00	PHYSPROP

mecloqualone C15H11ClN2O[9, 48, 64]



Compound Data

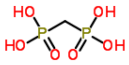
Melting point	**126.33 °C**	**399.48 K**			
CSID	9192	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	270.7136	**H bond donors**	0	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	Clc3ccccc3N/1C(=O)c2c(\N=C\1C)cccc2				
STD InChIKey	SFITWQDBYUMAPS-UHFFFAOYAG				

Melting Points

mp °C	source
126.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
126.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

127.00	PHYSPROP

medronic acid CH6O6P2[3, 64]



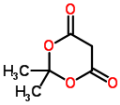
Compound Data

Melting point	**201.25 °C**	**474.40 K**			
CSID	15308	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	176.0023	**H bond donors**	4	**ACD/LogP**	-4.12
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	2.11 g/cm^3
SMILES	O=P(O)(O)CP(=O)(O)O				
STD InChIKey	MBKDYNNUVRNNRF-UHFFFAOYAP				

Melting Points

mp °C	source
203.00	Alfa Aesar
199.50	PHYSPROP

Meldrum's acid C6H8O4[3, 48, 64]



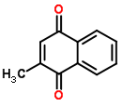
Compound Data

Melting point	**95.33 °C**	**368.48 K**			
CSID	15418	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	144.1253	**H bond donors**	0	**ACD/LogP**	-1.40
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	O=C1OC(OC(=O)C1)(C)C				
STD InChIKey	GXHFUVWIGNLZSC-UHFFFAOYAM				

Melting Points

mp °C	source
94.00	Alfa Aesar
98.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
94.00	PHYSPROP

menadione C11H8O2[3, 32, 61, 64]



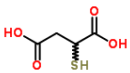
Compound Data

Melting point	**104.25 °C**	**377.40 K**			
CSID	3915	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	172.18	**H bond donors**	0	**ACD/LogP**	2.38
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3
SMILES	O=C\2c1c(cccc1)C(=O)/C(=C/2)C				
STD InChIKey	MJVAVZPDRWSRRC-UHFFFAOYAY				

Melting Points

mp °C	source
106.00	Alfa Aesar
102.00	DrugBank
102.00	Oxford University MSDS
107.00	PHYSPROP

mercaptosuccinic acid C4H6O4S[3, 64]



Compound Data

Melting point	**150.50 °C**	**423.65 K**			
CSID	6032	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	150.153	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.53 g/cm^3
SMILES	C(C(C(=O)O)S)C(=O)O				
STD InChIKey	NJRXVEJTAYWCQJ-UHFFFAOYAP				

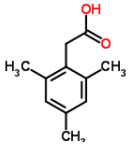
Melting Points

mp °C	source

152.00	Alfa Aesar
149.00	PHYSPROP

mesitylacetic acid C11H14O2[3, 47]

Compound Data



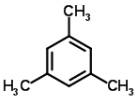
Melting point	**168.43 °C 441.57 K**				
CSID	70500	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	178.2277	**H bond donors**	1	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.07 g/cm^3
SMILES	O=C(O)Cc1c(cc(cc1C)C)C				
STD InChIKey	CQWMQAKKAHTCSC-UHFFFAOYAD				

Melting Points

mp °C	source
169.00	Alfa Aesar
167.85	IUCr

mesitylene C9H12[3, 4, 61, 64]

Compound Data



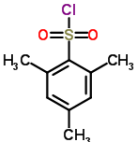
Melting point	**-44.92 °C 228.22 K**				
CSID	7659	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.1916	**H bond donors**	0	**ACD/LogP**	3.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	Cc1cc(cc(c1)C)C				
STD InChIKey	AUHZEENZYGFFBQ-UHFFFAOYAK				

Melting Points

mp °C	source
-45.00	Alfa Aesar
-45.00	American Petroleum Institute. Research Project 44; Selected ...
-45.00	Oxford University MSDS
-44.70	PHYSPROP

mesitylene-2-sulfonyl chloride C9H11ClO2S[3, 64]

Compound Data



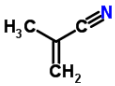
Melting point	**55.50 °C 328.65 K**				
CSID	12504	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	218.7004	**H bond donors**	0	**ACD/LogP**	3.37
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	O=S(Cl)(=O)c1c(cc(cc1C)C)C				
STD InChIKey	PVJZBZSCGJAWNG-UHFFFAOYAR				

Melting Points

mp °C	source
55.00	Alfa Aesar
56.00	PHYSPROP

methacrylonitrile C4H5N[2, 64]

Compound Data



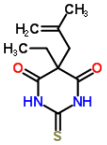
Melting point	**-35.90 °C 237.25 K**				
CSID	29101	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	67.0892	**H bond donors**	0	**ACD/LogP**	0.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.81 g/cm^3
SMILES	N#C\C(=C)C				
STD InChIKey	GYCMBHHDWRMZGG-UHFFFAOYAX				

Melting Points

mp °C	source

-36.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-35.80	PHYSPROP

methallatal C10H14N2O2S[9, 48, 64]



Compound Data

Melting point	**160.17 °C**	**433.32 K**			
CSID	2297301	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	226.2954	**H bond donors**	2	**ACD/LogP**	2.28
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	O=C1NC(=S)NC(=O)C1(CC)CC(=C)\C				
STD InChIKey	XMQICEWOKPEQRG-UHFFFAOYAA				

Melting Points

mp °C	source
160.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
160.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
160.50	PHYSPROP

methane CH4[59, 61, 64, 73]

Compound Data

Melting point	**-182.32 °C**	**90.83 K**			
CSID	291	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	16.0425	**H bond donors**	0	**ACD/LogP**	1.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.00 g/cm^3
SMILES	C				
STD InChIKey	VNWKTOKETHGBQD-UHFFFAOYAM				

Melting Points

mp °C	source
-182.55	NIST Web Book
-182.00	Oxford University MSDS
-182.40	PHYSPROP
	Values not used in calculating the average melting point
-187.45	Streng AG Journal of Chemical and Engineering Data 16(3) 357...[1]

1. Clearly out of Range - EC

methanethiol CH4S[61, 64]

Compound Data

Melting point	**-122.00 °C**	**151.15 K**			
CSID	855	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	48.1075	**H bond donors**	0	**ACD/LogP**	0.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.81 g/cm^3
SMILES	SC				
STD InChIKey	LSDPWZHWYPCBBB-UHFFFAOYAW				

Melting Points

mp °C	source
-121.00	Oxford University MSDS
-123.00	PHYSPROP

methanol CH4O[3, 3, 4, 19, 28, 61, 61, 64, 72]

Compound Data

Melting point	**-97.90 °C**	**175.25 K**			
CSID	864	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	32.0419	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.75 g/cm^3
SMILES	CO				

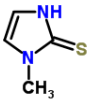
STD InChIKey	OKKJLVBELUTLKV-UHFFFAOYAX

Melting Points

mp °C	source
-98.00	Alfa Aesar
-98.00	Alfa Aesar
-98.00	American Petroleum Institute. Research Project 44; Selected ...
-98.00	Chemical Book
-97.53	CRC Handbook of Chemistry and Physics
-98.00	Oxford University MSDS
-98.00	Oxford University MSDS
-97.60	PHYSPROP
-98.00	Sigma-Aldrich

methimazole C4H6N2S[3, 28, 32, 56, 64, 72, 81, 84]

Compound Data



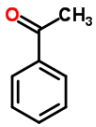
Melting point	**146.00 °C**	**419.15 K**			
CSID	1131173	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.1688	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.28 g/cm^3
SMILES	Cn1cc[nH]c1=S				
STD InChIKey	PMRYVIKBURPHAH-UHFFFAOYAN				

Melting Points

mp °C	source
146.00	Alfa Aesar
146.00	CRC Handbook of Chemistry and Physics
146.00	DrugBank
147.00	Merck Index
146.00	PHYSPROP
145.50	Sigma-Aldrich
146.00	Wikipedia
145.50	Wolfram Alpha

methimazole C8H8O[3, 8, 28, 31, 39, 61, 61, 64, 84]

Compound Data



Melting point	**19.73 °C**	**292.88 K**			
CSID	7132	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	120.1485	**H bond donors**	0	**ACD/LogP**	1.67
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.99 g/cm^3
SMILES	CC(=O)c1ccccc1				
STD InChIKey	KWOLFJPFCHCOCG-UHFFFAOYAT				

Melting Points

mp °C	source
20.00	Alfa Aesar
20.00	Bengston G.; Panek D.; Fritsch D. Journal of Membrane Scienc...
20.50	CRC Handbook of Chemistry and Physics
20.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
19.60	Ginzburg BM; Tuichiev Sh. Russian Journal of Applied Chemist...
19.00	Oxford University MSDS
19.00	Oxford University MSDS
20.00	PHYSPROP
19.50	Wolfram Alpha

methimazole C12H10[3, 44, 61, 64, 70]

Compound Data

Melting point	**94.28 °C**	**367.43 K**			
CSID	6478	**H bond acceptors**	0	**Rule of 5 violations**	0

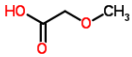
Molecular weight	154.2078	**H bond donors**	0	**ACD/LogP**	3.73
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	c1cc2cccc3c2c(c1)CC3				
STD InChIKey	CWRYPZZKDGJXCA-UHFFFAOYAW				

Melting Points

mp °C	source
94.00	Alfa Aesar
95.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
95.00	Oxford University MSDS
93.40	PHYSPROP
94.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

methoxyacetic acid C3H6O3[3, 35, 64]

Compound Data



Melting point	**7.80 °C**	**280.95 K**			
CSID	11750	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	90.0779	**H bond donors**	1	**ACD/LogP**	-0.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(O)COC				
STD InChIKey	RMIODHQZRUFFFF-UHFFFAOYAC				

Melting Points

mp °C	source
8.00	Alfa Aesar
7.70	EPISuite-ChemSpider
7.70	PHYSPROP

methoxyflurane C3H4Cl2F2O[3, 32, 61, 64]

Compound Data

Melting point	**-35.25 °C**	**237.90 K**			
CSID	3973	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	164.9661	**H bond donors**	0	**ACD/LogP**	1.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.39 g/cm^3
SMILES	ClC(Cl)C(F)(F)OC				
STD InChIKey	RFKMCNOHBTXSMU-UHFFFAOYAI				

Melting Points

mp °C	source
-36.00	Alfa Aesar
-35.00	DrugBank
-35.00	Oxford University MSDS
-35.00	PHYSPROP

methyl 2-amino-5-chlorobenzoate C8H8ClNO2[3, 64]

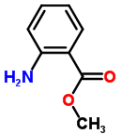
Compound Data

Melting point	**68.00 °C**	**341.15 K**			
CSID	71213	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	185.6076	**H bond donors**	2	**ACD/LogP**	2.92
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.31 g/cm^3
SMILES	Clc1cc(C(=O)OC)c(N)cc1				
STD InChIKey	IGHVUURTQGBABT-UHFFFAOYAW				

Melting Points

mp °C	source
69.00	Alfa Aesar
67.00	PHYSPROP

methyl 2-aminobenzoate C8H9NO2[2, 3, 61, 64]



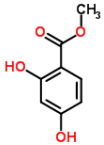
Compound Data

Melting point	**24.12 °C**	**297.27 K**			
CSID	13858096	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	2.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OC)c1ccccc1N				
STD InChIKey	VAMXMNNIEUEQDV-UHFFFAOYAV				

Melting Points

mp °C	source
24.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
24.00	Alfa Aesar
24.00	Oxford University MSDS
24.50	PHYSPROP

methyl 2,4-dihydroxybenzoate C8H8O4[3, 64]



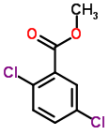
Compound Data

Melting point	**118.75 °C**	**391.90 K**			
CSID	15663	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	2	**ACD/LogP**	1.92
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.35 g/cm^3
SMILES	O=C(OC)c1ccc(O)cc1O				
STD InChIKey	IIFCLXHRIYTHPV-UHFFFAOYAU				

Melting Points

mp °C	source
118.00	Alfa Aesar
119.50	PHYSPROP

methyl 2,5-dichlorobenzoate C8H6Cl2O2[3, 64]



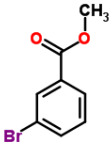
Compound Data

Melting point	**38.75 °C**	**311.90 K**			
CSID	16951	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	205.038	**H bond donors**	0	**ACD/LogP**	3.06
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.35 g/cm^3
SMILES	O=C(OC)c1cc(Cl)ccc1Cl				
STD InChIKey	SPJQBGGHUDNAIC-UHFFFAOYAB				

Melting Points

mp °C	source
39.00	Alfa Aesar
38.50	PHYSPROP

methyl 3-bromobenzoate C8H7BrO2[3, 7, 64]



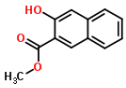
Compound Data

Melting point	**32.33 °C**	**305.48 K**			
CSID	11573	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	215.044	**H bond donors**	0	**ACD/LogP**	2.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.50 g/cm^3
SMILES	O=C(OC)c1cc(Br)ccc1				
STD InChIKey	KMFJVYMFCAIRAN-UHFFFAOYAT				

Melting Points

mp °C	source
32.00	Alfa Aesar
33.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
32.00	PHYSPROP

methyl 3-hydroxy-2-naphthoate C12H10O3[3, 64]



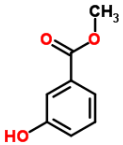
Compound Data

Melting point	**74.25 °C**	**347.40 K**			
CSID	63350	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	202.206	**H bond donors**	1	**ACD/LogP**	3.46
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.26 g/cm^3
SMILES	O=C(OC)c2cc1c(cccc1)cc2O				
STD InChIKey	YVVBECLPRBAATK-UHFFFAOYAT				

Melting Points

mp °C	source
73.00	Alfa Aesar
75.50	PHYSPROP

methyl 3-hydroxybenzoate C8H8O3[2, 3, 64]



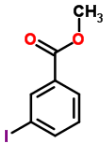
Compound Data

Melting point	**72.67 °C**	**345.82 K**			
CSID	79453	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	O=C(OC)c1cc(O)ccc1				
STD InChIKey	YKUCHDXIBAQWSF-UHFFFAOYAO				

Melting Points

mp °C	source
74.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
71.00	Alfa Aesar
73.00	PHYSPROP

methyl 3-nitrobenzoate C8H7IO2[7, 64]



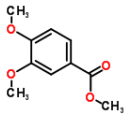
Compound Data

Melting point	**54.25 °C**	**327.40 K**			
CSID	62471	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	262.0444	**H bond donors**	0	**ACD/LogP**	3.31
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.75 g/cm^3
SMILES	O=C(OC)c1cc(I)ccc1				
STD InChIKey	NPXOIGSBRLCOSD-UHFFFAOYAY				

Melting Points

mp °C	source
54.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
54.50	PHYSPROP

methyl 3,4-dimethoxybenzoate C10H12O4[2, 3, 64]



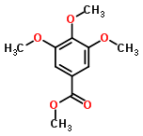
Compound Data

Melting point	**59.93 °C**	**333.08 K**			
CSID	21159598	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	196.1999	**H bond donors**	0	**ACD/LogP**	2.06
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.12 g/cm^3
SMILES	COc1cc(ccc1OC)C(=O)OC				
STD InChIKey	BIGQPYZPEWAPBG-UHFFFAOYAL				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
59.00	Alfa Aesar
60.80	PHYSPROP

methyl 3,4,5-trimethoxybenzoate C11H14O5[2, 3, 48, 64]



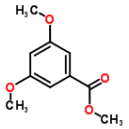
Compound Data

Melting point	**83.75 °C**	**356.90 K**			
CSID	15161	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	226.2259	**H bond donors**	0	**ACD/LogP**	1.74
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.13 g/cm^3
SMILES	O=C(OC)c1cc(OC)c(OC)c(OC)c1				
STD InChIKey	KACHFMOHOPLTNX-UHFFFAOYAF				

Melting Points

mp °C	source
84.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
83.00	Alfa Aesar
85.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
83.00	PHYSPROP

methyl 3,5-dimethoxybenzoate C10H12O4[2, 3]



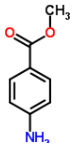
Compound Data

Melting point	**42.50 °C**	**315.65 K**			
CSID	21159597	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	196.1999	**H bond donors**	0	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.12 g/cm^3
SMILES	COc1cc(cc(OC)c1)C(=O)OC				
STD InChIKey	YXUIOVUOFQKWDM-UHFFFAOYAR				

Melting Points

mp °C	source
43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
42.00	Alfa Aesar

methyl 4-aminobenzoate C8H9NO2[3, 64, 70, 72]



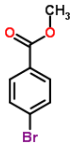
Compound Data

Melting point	**111.75 °C**	**384.90 K**			
CSID	11585	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	1.41
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=C(OC)c1ccc(N)cc1				
STD InChIKey	LZXXNPOYQCLXRS-UHFFFAOYAA				

Melting Points

mp °C	source
112.00	Alfa Aesar
110.50	PHYSPROP
114.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
110.50	Sigma-Aldrich

methyl 4-bromobenzoate C8H7BrO2[3, 7, 64]



Compound Data

Melting point	**80.33 °C**	**353.48 K**			
CSID	11584	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	215.044	**H bond donors**	0	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.50 g/cm^3
SMILES	O=C(OC)c1ccc(Br)cc1				
STD InChIKey	CZNGTXVOZOWWKM-UHFFFAOYAF				

Melting Points

mp °C	source

79.00	Alfa Aesar
81.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
81.00	PHYSPROP

methyl 4-chloro-3-nitrobenzoate C8H6ClNO4[3, 64]

Compound Data

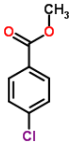
Melting point	**81.50 °C**	**354.65 K**			
CSID	642951	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	215.5905	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.43 g/cm^3
SMILES	O=[N+]([O-])c1cc(ccc1Cl)C(=O)OC				
STD InChIKey	XRTKWPWDSUNLHS-UHFFFAOYAD				

Melting Points

mp °C	source
80.00	Alfa Aesar
83.00	PHYSPROP

methyl 4-chlorobenzoate C8H7ClO2[2, 3, 64]

Compound Data



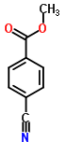
Melting point	**43.50 °C**	**316.65 K**			
CSID	13669	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	170.593	**H bond donors**	0	**ACD/LogP**	2.76
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.22 g/cm^3
SMILES	O=C(OC)c1ccc(Cl)cc1				
STD InChIKey	LXNFVVDCCWUUKC-UHFFFAOYAM				

Melting Points

mp °C	source
44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
43.00	Alfa Aesar
43.50	PHYSPROP

methyl 4-cyanobenzoate C9H7NO2[3, 7, 48]

Compound Data



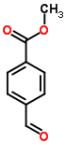
Melting point	**63.67 °C**	**336.82 K**			
CSID	63956	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	161.1574	**H bond donors**	0	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	N#Cc1ccc(C(=O)OC)cc1				
STD InChIKey	KKZMIDYKRKGJHG-UHFFFAOYAA				

Melting Points

mp °C	source
67.00	Alfa Aesar
62.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
62.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

methyl 4-formylbenzoate C9H8O3[2, 3, 61]

Compound Data



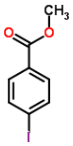
Melting point	**60.67 °C**	**333.82 K**			
CSID	14559	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	164.158	**H bond donors**	0	**ACD/LogP**	2.05
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.18 g/cm^3
SMILES	O=C(OC)c1ccc(C=O)cc1				
STD InChIKey	FEIOASZZURHTHB-UHFFFAOYAD				

Melting Points

mp °C	source
60.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
61.00	Alfa Aesar
61.00	Oxford University MSDS

methyl 4-iodobenzoate C8H7IO2[3, 7, 64]

Compound Data



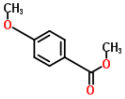
Melting point	**114.93 °C**	**388.08 K**			
CSID	62484	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	262.0444	**H bond donors**	0	**ACD/LogP**	3.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.75 g/cm^3
SMILES	O=C(OC)c1ccc(I)cc1				
STD InChIKey	DYUWQWMXZHDZOR-UHFFFAOYAE				

Melting Points

mp °C	source
115.00	Alfa Aesar
115.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
114.80	PHYSPROP

methyl 4-methoxybenzoate C9H10O3[2, 3, 64]

Compound Data



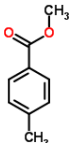
Melting point	**49.67 °C**	**322.82 K**			
CSID	21108577	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	0	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(OC)c1ccc(OC)cc1				
STD InChIKey	DDIZAANNODHTRB-UHFFFAOYAF				

Melting Points

mp °C	source
50.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
50.00	Alfa Aesar
49.00	PHYSPROP

methyl 4-methylbenzoate C9H10O2[2, 3, 64]

Compound Data



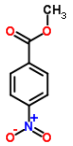
Melting point	**34.73 °C**	**307.88 K**			
CSID	7175	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	150.1745	**H bond donors**	0	**ACD/LogP**	2.66
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	O=C(OC)c1ccc(cc1)C				
STD InChIKey	QSSJZLPUHJDYKF-UHFFFAOYAH				

Melting Points

mp °C	source
37.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
34.00	Alfa Aesar
33.20	PHYSPROP

methyl 4-nitrobenzoate C8H7NO4[2, 3, 64]

Compound Data



Melting point	**95.67 °C**	**368.82 K**			
CSID	11586	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	181.1455	**H bond donors**	0	**ACD/LogP**	1.80
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.30 g/cm^3
SMILES	O=[N+]([O-])c1ccc(C(=O)OC)cc1				

STD InChIKey	YOJAHJGBFDPSDI-UHFFFAOYAX

Melting Points

mp °C	source
96.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
96.00	Alfa Aesar
95.00	PHYSPROP

methyl 5-chloro-2-hydroxybenzoate C8H7ClO3[3, 64]

Compound Data

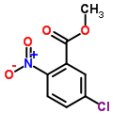
Melting point	**48.00 °C**	**321.15 K**			
CSID	70085	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	186.5924	**H bond donors**	1	**ACD/LogP**	3.24
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.35 g/cm^3
SMILES	Clc1cc(C(=O)OC)c(O)cc1				
STD InChIKey	KJWHRMZKJXOWFC-UHFFFAOYAE				

Melting Points

mp °C	source
46.00	Alfa Aesar
50.00	PHYSPROP

methyl 5-chloro-2-nitrobenzoate C8H6ClNO4[3, 64]

Compound Data



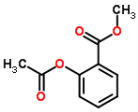
Melting point	**48.75 °C**	**321.90 K**			
CSID	149513	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	215.5905	**H bond donors**	0	**ACD/LogP**	2.37
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.43 g/cm^3
SMILES	O=[N+]([O-])c1c(cc(Cl)cc1)C(=O)OC				
STD InChIKey	JGBJHRKCUKTQOE-UHFFFAOYAV				

Melting Points

mp °C	source
49.00	Alfa Aesar
48.50	PHYSPROP

methyl acetylsalicylate C10H10O4[7, 64]

Compound Data



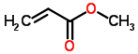
Melting point	**51.75 °C**	**324.90 K**			
CSID	61759	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	1.47
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=C(Oc1ccccc1C(=O)OC)C				
STD InChIKey	ONWPLBKWMAUFGZ-UHFFFAOYAR				

Melting Points

mp °C	source
52.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
51.50	PHYSPROP

methyl acrylate C4H6O2[2, 3, 61, 64]

Compound Data



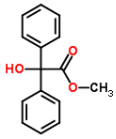
Melting point	**-75.38 °C**	**197.77 K**			
CSID	7022	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	86.0892	**H bond donors**	0	**ACD/LogP**	0.79
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.92 g/cm^3
SMILES	COC(=O)C=C				
STD InChIKey	BAPJBEWLBFYGME-UHFFFAOYAO				

Melting Points

mp °C	source
-75.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-75.00	Alfa Aesar
-75.00	Oxford University MSDS
-76.50	PHYSPROP

methyl benzilate C15H14O3[3, 64]

Compound Data



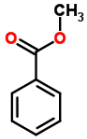
Melting point	**75.40 °C**	**348.55 K**			
CSID	59546	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	242.2699	**H bond donors**	1	**ACD/LogP**	3.01
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.19 g/cm^3
SMILES	O=C(OC)C(O)(c1ccccc1)c2ccccc2				
STD InChIKey	LJFIHTFNTGQZJL-UHFFFAOYAO				

Melting Points

mp °C	source
75.00	Alfa Aesar
75.80	PHYSPROP

methyl benzoate C8H8O2[3, 31, 61, 64]

Compound Data



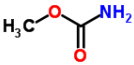
Melting point	**-12.75 °C**	**260.40 K**			
CSID	6883	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	0	**ACD/LogP**	2.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.07 g/cm^3
SMILES	O=C(OC)c1ccccc1				
STD InChIKey	QPJVMBTYPHYUOC-UHFFFAOYAK				

Melting Points

mp °C	source
-12.00	Alfa Aesar
-12.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-12.00	Oxford University MSDS
-15.00	PHYSPROP

methyl carbamate C2H5NO2[3, 64]

Compound Data



Melting point	**54.50 °C**	**327.65 K**			
CSID	11229	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	75.0666	**H bond donors**	2	**ACD/LogP**	-0.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.09 g/cm^3
SMILES	O=C(OC)N				
STD InChIKey	GTCAXTIRRLKXRU-UHFFFAOYAJ				

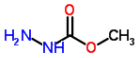
Melting Points

mp °C	source
55.00	Alfa Aesar
54.00	PHYSPROP

methyl carbazate C2H6N2O2[3, 48, 64]

Compound Data

Melting point	**72.33 °C**	**345.48 K**			
CSID	72718	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	90.0812	**H bond donors**	3	**ACD/LogP**	-0.79
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.16 g/cm^3



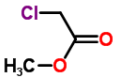
SMILES	O=C(OC)NN
STD InChIKey	WFJRIDQGVSJLLH-UHFFFAOYAE

Melting Points

mp °C	source
72.00	Alfa Aesar
72.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
73.00	PHYSPROP

methyl chloroacetate C3H5ClO2[3, 64]

Compound Data



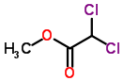
Melting point	**-32.05 °C**	**241.10 K**			
CSID	13872667	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.5236	**H bond donors**	0	**ACD/LogP**	0.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	ClCC(=O)OC				
STD InChIKey	QABLOFMHHSOFRJ-UHFFFAOYAJ				

Melting Points

mp °C	source
-32.00	Alfa Aesar
-32.10	PHYSPROP

methyl dichloroacetate C3H4Cl2O2[3, 64]

Compound Data



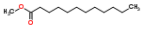
Melting point	**-51.95 °C**	**221.20 K**			
CSID	8013	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	142.9687	**H bond donors**	0	**ACD/LogP**	0.99
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.36 g/cm^3
SMILES	ClC(Cl)C(=O)OC				
STD InChIKey	HKMLRUAPIDAGIE-UHFFFAOYAG				

Melting Points

mp °C	source
-52.00	Alfa Aesar
-51.90	PHYSPROP

methyl dodecanoate C13H26O2[3, 64]

Compound Data



Melting point	**5.10 °C**	**278.25 K**			
CSID	7847	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	214.3443	**H bond donors**	0	**ACD/LogP**	5.49
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.87 g/cm^3
SMILES	O=C(OC)CCCCCCCCCCC				
STD InChIKey	UQDUPQYQJKYHQI-UHFFFAOYAP				

Melting Points

mp °C	source
5.00	Alfa Aesar
5.20	PHYSPROP

methyl formate C2H4O2[2, 3, 61, 64]

Compound Data

Melting point	**-99.75 °C**	**173.40 K**

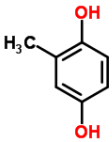
CSID	7577	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	60.052	**H bond donors**	0	**ACD/LogP**	-0.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.92 g/cm^3
SMILES	O=COC				
STD InChIKey	TZIHFWKZFHZASV-UHFFFAOYAI				

Melting Points

mp °C	source
-100.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-100.00	Alfa Aesar
-100.00	Oxford University MSDS
-99.00	PHYSPROP

methyl hydroquinone C7H8O2[3, 61, 64]

Compound Data



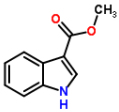
Melting point	**128.67 °C**	**401.82 K**			
CSID	6983	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	1.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.21 g/cm^3
SMILES	Oc1ccc(O)c(c1)C				
STD InChIKey	CNHDIAIOKMXOLK-UHFFFAOYAG				

Melting Points

mp °C	source
129.00	Alfa Aesar
129.00	Oxford University MSDS
128.00	PHYSPROP

methyl indole-3-carboxylate C10H9NO2[3, 64]

Compound Data



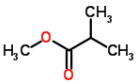
Melting point	**150.75 °C**	**423.90 K**			
CSID	512092	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	175.184	**H bond donors**	1	**ACD/LogP**	2.54
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	COC(=O)c2cnc1ccccc12				
STD InChIKey	QXAUTQFAWKKNLM-UHFFFAOYAU				

Melting Points

mp °C	source
151.00	Alfa Aesar
150.50	PHYSPROP

methyl isobutyrate C5H10O2[3, 64]

Compound Data

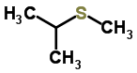


Melting point	**-84.85 °C**	**188.30 K**			
CSID	10571	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	0	**ACD/LogP**	1.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.89 g/cm^3
SMILES	O=C(OC)C(C)C				
STD InChIKey	BHIWKHZACMWKOJ-UHFFFAOYAO				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-84.70	PHYSPROP

methyl isopropyl sulfide C4H10S[4, 64]



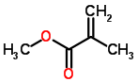
Compound Data

Melting point	**-101.75 °C**	**171.40 K**			
CSID	14512	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	90.1872	**H bond donors**	0	**ACD/LogP**	1.77
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.83 g/cm^3
SMILES	S(C(C)C)C				
STD InChIKey	ROSSIHMZZJOVOU-UHFFFAOYAD				

Melting Points

mp °C	source
-102.00	American Petroleum Institute. Research Project 44; Selected ...
-101.50	PHYSPROP

methyl methacrylate C5H8O2[2, 3, 61, 64]



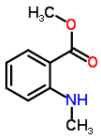
Compound Data

Melting point	**-47.89 °C**	**225.26 K**			
CSID	6406	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	100.1158	**H bond donors**	0	**ACD/LogP**	1.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.91 g/cm^3
SMILES	O=C(OC)\C(=C)C				
STD InChIKey	VVQNEPGJFQJSBK-UHFFFAOYAN				

Melting Points

mp °C	source
-48.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-48.00	Alfa Aesar
-48.00	Oxford University MSDS
-47.55	PHYSPROP

methyl N-methylanthranilate C9H11NO2[3, 64]



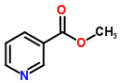
Compound Data

Melting point	**18.50 °C**	**291.65 K**			
CSID	21108245	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	165.1891	**H bond donors**	1	**ACD/LogP**	2.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.12 g/cm^3
SMILES	CNc1ccccc1C(=O)OC				
STD InChIKey	GVOWHGSUZUUUDR-UHFFFAOYAS				

Melting Points

mp °C	source
18.00	Alfa Aesar
19.00	PHYSPROP

methyl nicotinate C7H7NO2[3, 64]



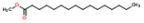
Compound Data

Melting point	**42.25 °C**	**315.40 K**			
CSID	21111785	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	0	**ACD/LogP**	0.88
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(OC)c1cccnc1				
STD InChIKey	YNBADRVTZLEFNH-UHFFFAOYAU				

Melting Points

mp °C	source
42.00	Alfa Aesar
42.50	PHYSPROP

methyl palmitate C17H34O2[3, 64]



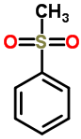
Compound Data

Melting point	**30.50 °C**	**303.65 K**			
CSID	7889	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	270.4507	**H bond donors**	0	**ACD/LogP**	7.62
Phase 25 °C	solid	**Rotatable bonds**	15	**Predicted density**	0.86 g/cm^3
SMILES	O=C(OC)CCCCCCCCCCCCCCC				
STD InChIKey	FLIACVVOZYBSBS-UHFFFAOYAK				

Melting Points

mp °C	source
31.00	Alfa Aesar
30.00	PHYSPROP

methyl phenyl sulfone C7H8O2S[3, 64]



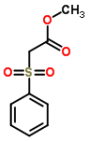
Compound Data

Melting point	**86.50 °C**	**359.65 K**			
CSID	17347	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	156.2022	**H bond donors**	0	**ACD/LogP**	0.50
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.19 g/cm^3
SMILES	O=S(=O)(c1ccccc1)C				
STD InChIKey	JCDWETOKTFWTHA-UHFFFAOYAQ				

Melting Points

mp °C	source
87.00	Alfa Aesar
86.00	PHYSPROP

methyl phenylsulfonylacetate C9H10O4S[3, 64]



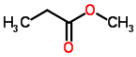
Compound Data

Melting point	**32.50 °C**	**305.65 K**			
CSID	483123	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	214.2383	**H bond donors**	0	**ACD/LogP**	0.70
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.28 g/cm^3
SMILES	COC(=O)CS(=O)(=O)c1ccccc1				
STD InChIKey	NLEAIFBNKPYTGN-UHFFFAOYAT				

Melting Points

mp °C	source
30.00	Alfa Aesar
35.00	PHYSPROP

methyl propionate C4H8O2[2, 3, 61, 64]



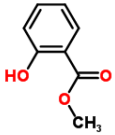
Compound Data

Melting point	**-87.88 °C**	**185.27 K**			
CSID	10653	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	0	**ACD/LogP**	0.71
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.90 g/cm^3
SMILES	O=C(OC)CC				
STD InChIKey	RJUFJBKOKNCXHH-UHFFFAOYAS				

Melting Points

mp °C	source
-88.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-88.00	Alfa Aesar
-88.00	Oxford University MSDS
-87.50	PHYSPROP

methyl salicylate C8H8O3[2, 3, 61, 64]



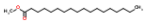
Compound Data

Melting point	**-8.25 °C**	**264.90 K**			
CSID	13848808	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	2.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	O=C(OC)c1ccccc1O				
STD InChIKey	OSWPMRLSEDHDFF-UHFFFAOYAD				

Melting Points

mp °C	source
-7.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-9.00	Alfa Aesar
-9.00	Oxford University MSDS
-8.00	PHYSPROP

methyl stearate C19H38O2[3, 64]



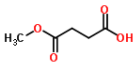
Compound Data

Melting point	**39.55 °C**	**312.70 K**			
CSID	7909	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	298.5038	**H bond donors**	0	**ACD/LogP**	8.68
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.86 g/cm^3
SMILES	O=C(OC)CCCCCCCCCCCCCCCCC				
STD InChIKey	HPEUJPJOZXNMSJ-UHFFFAOYAE				

Melting Points

mp °C	source
40.00	Alfa Aesar
39.10	PHYSPROP

methyl succinate C5H8O4[61, 64]



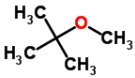
Compound Data

Melting point	**57.75 °C**	**330.90 K**			
CSID	69896	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	132.1146	**H bond donors**	1	**ACD/LogP**	-0.21
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.21 g/cm^3
SMILES	O=C(O)CCC(=O)OC				
STD InChIKey	JDRMYOQETPMYQX-UHFFFAOYAV				

Melting Points

mp °C	source
57.50	Oxford University MSDS
58.00	PHYSPROP

methyl t-butyl ether C5H12O[3, 4, 61, 64]



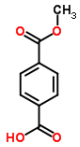
Compound Data

Melting point	**-108.90 °C**	**164.25 K**			
CSID	14672	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	0	**ACD/LogP**	1.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.75 g/cm^3
SMILES	O(C(C)(C)C)C				
STD InChIKey	BZLVMXJERCGZMT-UHFFFAOYAA				

Melting Points

mp °C	source
-109.00	Alfa Aesar
-109.00	American Petroleum Institute. Research Project 44; Selected ...
-109.00	Oxford University MSDS
-108.60	PHYSPROP

methyl terephthalate C9H8O4[2, 64]



Compound Data

Melting point	**221.50 °C**	**494.65 K**			
CSID	14760	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	180.1574	**H bond donors**	1	**ACD/LogP**	2.30
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.29 g/cm^3
SMILES	O=C(OC)c1ccc(C(=O)O)cc1				
STD InChIKey	REIDAMBAPLIATC-UHFFFAOYAP				

Melting Points

mp °C	source
221.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
222.00	PHYSPROP

methyl tetradecanoate C15H30O2[3, 64]

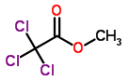
Compound Data

Melting point	**18.50 °C**	**291.65 K**			
CSID	29024	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	242.3975	**H bond donors**	0	**ACD/LogP**	6.55
Phase 25 °C	liquid/gas	**Rotatable bonds**	13	**Predicted density**	0.87 g/cm^3
SMILES	O=C(OC)CCCCCCCCCCCCC				
STD InChIKey	ZAZKJZBWRNNLDS-UHFFFAOYAX				

Melting Points

mp °C	source
18.00	Alfa Aesar
19.00	PHYSPROP

methyl trichloroacetate C3H3Cl3O2[3, 64]



Compound Data

Melting point	**-17.75 °C**	**255.40 K**			
CSID	11246	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	177.4137	**H bond donors**	0	**ACD/LogP**	2.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.53 g/cm^3
SMILES	ClC(Cl)(Cl)C(=O)OC				
STD InChIKey	VHFUHRXYRYWELT-UHFFFAOYAW				

Melting Points

mp °C	source
-18.00	Alfa Aesar
-17.50	PHYSPROP

methylamine CH5N[61, 64]

Compound Data

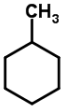
Melting point	**-93.20 °C**	**179.95 K**			
CSID	6089	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	31.0571	**H bond donors**	2	**ACD/LogP**	-0.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.64 g/cm^3
SMILES	NC				
STD InChIKey	BAVYZALUXZFZLV-UHFFFAOYAN				

Melting Points

mp °C	source
-93.00	Oxford University MSDS
-93.40	PHYSPROP

methylcyclohexane C7H14[3, 4, 61, 64]

Compound Data



Melting point	**-126.65 °C**	**146.50 K**			
CSID	7674	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	98.1861	**H bond donors**	0	**ACD/LogP**	3.70
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.78 g/cm^3
SMILES	CC1CCCCC1				
STD InChIKey	UAEPNZWRGJTJPN-UHFFFAOYAG				

Melting Points

mp °C	source
-126.00	Alfa Aesar
-127.00	American Petroleum Institute. Research Project 44; Selected ...
-127.00	Oxford University MSDS
-126.60	PHYSPROP

methylcyclopentane C6H12[3, 4, 64]

Compound Data

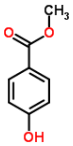
Melting point	**-142.50 °C**	**130.65 K**			
CSID	7024	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.31
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3
SMILES	CC1CCCC1				
STD InChIKey	GDOPTJXRTPNYNR-UHFFFAOYAS				

Melting Points

mp °C	source
-143.00	Alfa Aesar
-142.00	American Petroleum Institute. Research Project 44; Selected ...
-142.50	PHYSPROP

methylparaben C8H8O3[2, 3, 35, 44, 61, 64, 70]

Compound Data



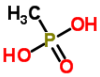
Melting point	**129.43 °C**	**402.58 K**			
CSID	7176	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	COC(=O)c1ccc(cc1)O				
STD InChIKey	LXCFILQKKLGQFO-UHFFFAOYAH				

Melting Points

mp °C	source
128.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
127.00	Alfa Aesar
131.00	EPISuite-ChemSpider
131.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
127.00	Oxford University MSDS
131.00	PHYSPROP
131.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

methylphosphonic acid CH5O3P[3, 61, 64]

Compound Data



Melting point	**106.50 °C**	**379.65 K**			
CSID	13220	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	96.0224	**H bond donors**	2	**ACD/LogP**	-2.02
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.50 g/cm^3
SMILES	O=P(O)(O)C				
STD InChIKey	YACKEPLHDIMKIO-UHFFFAOYAB				

Melting Points

mp °C	source

105.00	Alfa Aesar
106.00	Oxford University MSDS
108.50	PHYSPROP

methylphosphonic dichloride CH3Cl2OP[61, 64]

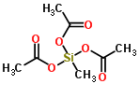
Compound Data

Melting point	**35.50 °C**	**308.65 K**			
CSID	12150	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	132.9137	**H bond donors**	0	**ACD/LogP**	0.26
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.45 g/cm^3
SMILES	ClP(Cl)(=O)C				
STD InChIKey	SCLFRABIDYGTAZ-UHFFFAOYAS				

Melting Points

mp °C	source
35.00	Oxford University MSDS
36.00	PHYSPROP

methyltriacetoxysilane C7H12O6Si[3, 64]



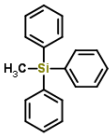
Compound Data

Melting point	**41.75 °C**	**314.90 K**			
CSID	70319	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	220.2521	**H bond donors**	0	**ACD/LogP**	1.37
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.16 g/cm^3
SMILES	O=C(O[Si](OC(=O)C)(OC(=O)C)C)C				
STD InChIKey	TVJPBVNWVPUZBM-UHFFFAOYAG				

Melting Points

mp °C	source
43.00	Alfa Aesar
40.50	PHYSPROP

methyltriphenylsilane C19H18Si[3, 64]



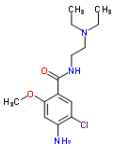
Compound Data

Melting point	**68.25 °C**	**341.40 K**			
CSID	455964	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	274.4317	**H bond donors**	0	**ACD/LogP**	6.42
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.04 g/cm^3
SMILES	c1(ccccc1)[Si](c2ccccc2)(c3ccccc3)C				
STD InChIKey	GIGVICQLYWGMGW-UHFFFAOYAN				

Melting Points

mp °C	source
67.00	Alfa Aesar
69.50	PHYSPROP

metoclopramide C14H22ClN3O2[9, 32, 44, 48, 64]



Compound Data

Melting point	**147.16 °C**	**420.31 K**			
CSID	4024	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	299.7964	**H bond donors**	3	**ACD/LogP**	2.22
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.16 g/cm^3
SMILES	Clc1cc(c(OC)cc1N)C(=O)NCCN(CC)CC				
STD InChIKey	TTWJBBZEZQICBI-UHFFFAOYAD				

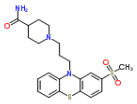
Melting Points

mp °C	source
147.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...

147.25	DrugBank
147.30	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
147.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
147.25	PHYSPROP

metopimazine C22H27N3O3S2[9, 64]

Compound Data



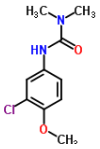
Melting point	**170.25 °C**	**443.40 K**			
CSID	24584	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	445.5981	**H bond donors**	2	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.29 g/cm^3
SMILES	O=S(=O)(c2cc1N(c3c(Sc1cc2)cccc3)CCCN4CCC(C(=O)N)CC4)C				
STD InChIKey	BQDBKDMTIJBJLA-UHFFFAOYAM				

Melting Points

mp °C	source
170.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
170.50	PHYSPROP

metoxuran C10H13ClN2O2[64, 70]

Compound Data



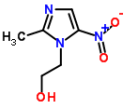
Melting point	**126.75 °C**	**399.90 K**			
CSID	27749	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	228.6754	**H bond donors**	1	**ACD/LogP**	1.80
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	Clc1cc(ccc1OC)NC(=O)N(C)C				
STD InChIKey	DSRNRYQBBJQVCW-UHFFFAOYAL				

Melting Points

mp °C	source
126.50	PHYSPROP
127.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

metronidazole C6H9N3O3[32, 44, 61, 70]

Compound Data



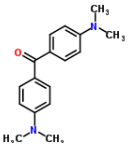
Melting point	**159.75 °C**	**432.90 K**			
CSID	4029	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	171.154	**H bond donors**	1	**ACD/LogP**	-0.01
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.45 g/cm^3
SMILES	[O-][N+](=O)c1cnc(n1CCO)C				
STD InChIKey	VAOCPAMSLUNLGC-UHFFFAOYAG				

Melting Points

mp °C	source
160.00	DrugBank
159.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
160.00	Oxford University MSDS
160.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

Michler's ketone C17H20N2O[3, 64]

Compound Data



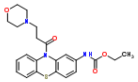
Melting point	**177.00 °C**	**450.15 K**			
CSID	6764	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	268.3535	**H bond donors**	0	**ACD/LogP**	3.87
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.10 g/cm^3
SMILES	O=C(c1ccc(N(C)C)cc1)c2ccc(N(C)C)cc2				
STD InChIKey	VVBLNCFGVYUYGU-UHFFFAOYAE				

Melting Points

mp °C	source
175.00	Alfa Aesar
179.00	PHYSPROP

moricizine C22H25N3O4S[9, 32, 48, 64]

Compound Data



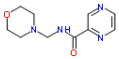
Melting point	**156.25 °C**	**429.40 K**			
CSID	31872	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	427.5166	**H bond donors**	1	**ACD/LogP**	2.33
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.31 g/cm^3
SMILES	O=C(OCC)Nc2cc1N(c3c(Sc1cc2)cccc3)C(=O)CCN4CCOCC4				
STD InChIKey	FUBVWMNBEHXPSU-UHFFFAOYAD				

Melting Points

mp °C	source
156.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
156.50	DrugBank
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
156.50	PHYSPROP

morphazinamide C10H14N4O2[9, 64]

Compound Data



Melting point	**118.75 °C**	**391.90 K**			
CSID	63555	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	222.2438	**H bond donors**	1	**ACD/LogP**	-1.07
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	O=C(NCN1CCOCC1)c2nccnc2				
STD InChIKey	GVTLAVKAVSKBKK-UHFFFAOYAT				

Melting Points

mp °C	source
119.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
118.50	PHYSPROP

morpholine C4H9NO[3, 61, 64]

Compound Data

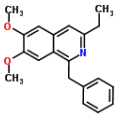
Melting point	**-4.93 °C**	**268.22 K**			
CSID	13837537	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	87.1204	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.93 g/cm^3
SMILES	C1CNCCO1				
STD InChIKey	YNAVUWVOSKDBBP-UHFFFAOYAU				

Melting Points

mp °C	source
-5.00	Alfa Aesar
-5.00	Oxford University MSDS
-4.80	PHYSPROP

moxaverine C20H21NO2[9, 48, 64]

Compound Data



Melting point	**78.17 °C**	**351.32 K**			
CSID	64045	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	307.3862	**H bond donors**	0	**ACD/LogP**	5.00
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.11 g/cm^3
SMILES	O(c1cc2c(cc1OC)cc(nc2Cc3ccccc3)CC)C				

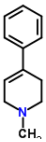
STD InChIKey	MYCMTMIGRXJNSO-UHFFFAOYAK

Melting Points

mp °C	source
78.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
78.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
78.50	PHYSPROP

MPTP C12H15N[61, 64]

Compound Data



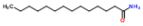
Melting point	**39.25 °C**	**312.40 K**			
CSID	1346	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	173.2542	**H bond donors**	0	**ACD/LogP**	2.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.00 g/cm^3
SMILES	c2c(/C1=C/CN(C)CC1)cccc2				
STD InChIKey	PLRACCBDVIHHLZ-UHFFFAOYAV				

Melting Points

mp °C	source
38.50	Oxford University MSDS
40.00	PHYSPROP

myristamide C14H29NO[3, 64]

Compound Data



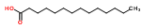
Melting point	**105.00 °C**	**378.15 K**			
CSID	62698	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	227.3862	**H bond donors**	2	**ACD/LogP**	5.14
Phase 25 °C	solid	**Rotatable bonds**	12	**Predicted density**	0.87 g/cm^3
SMILES	O=C(N)CCCCCCCCCCCCC				
STD InChIKey	QEALYLRSRQDCRA-UHFFFAOYAT				

Melting Points

mp °C	source
106.00	Alfa Aesar
104.00	PHYSPROP

myristic acid C14H28O2[3, 61, 64]

Compound Data



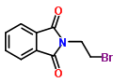
Melting point	**54.67 °C**	**327.82 K**			
CSID	10539	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	228.3709	**H bond donors**	1	**ACD/LogP**	5.79
Phase 25 °C	solid	**Rotatable bonds**	12	**Predicted density**	0.90 g/cm^3
SMILES	CCCCCCCCCCCCCC(=O)O				
STD InChIKey	TUNFSRHWOTWDNC-UHFFFAOYAZ				

Melting Points

mp °C	source
55.00	Alfa Aesar
55.10	Oxford University MSDS
53.90	PHYSPROP

N-(2-bromoethyl)phthalimide C10H8BrNO2[3, 64]

Compound Data



Melting point	**82.25 °C**	**355.40 K**			
CSID	10848	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	254.08	**H bond donors**	0	**ACD/LogP**	2.53
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.66 g/cm^3
SMILES	O=C2c1ccccc1C(=O)N2CCBr				

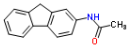
STD InChIKey	CHZXTOCAICMPQR-UHFFFAOYAF

Melting Points

mp °C	source
82.00	Alfa Aesar
82.50	PHYSPROP

N-(2-fluorenyl)acetamide C15H13NO[61, 64]

Compound Data



Melting point	**193.50 °C**	**466.65 K**			
CSID	5686	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	223.2698	**H bond donors**	1	**ACD/LogP**	3.03
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.23 g/cm^3
SMILES	O=C(Nc3ccc2c1ccccc1Cc2c3)C				
STD InChIKey	CZIHNRWJTSTCEX-UHFFFAOYAF				

Melting Points

mp °C	source
194.00	Oxford University MSDS
193.00	PHYSPROP

N-(2-hydroxyphenyl)acetamide C8H9NO2[2, 3, 61, 64]

Compound Data

Melting point	**207.00 °C**	**480.15 K**			
CSID	11477	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	151.1626	**H bond donors**	2	**ACD/LogP**	0.72
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.25 g/cm^3
SMILES	O=C(Nc1ccccc1O)C				
STD InChIKey	ADVGKWPZRIDURE-UHFFFAOYAG				

Melting Points

mp °C	source
207.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
208.00	Alfa Aesar
205.00	Oxford University MSDS
208.00	PHYSPROP

n-(2-nitrophenyl)acetamide C8H8N2O3[3, 64]

Compound Data

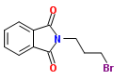
Melting point	**93.00 °C**	**366.15 K**			
CSID	10619	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	180.1607	**H bond donors**	1	**ACD/LogP**	1.00
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.34 g/cm^3
SMILES	O=C(Nc1ccccc1[N+]([O-])=O)C				
STD InChIKey	BUNFNRVLMKHKIT-UHFFFAOYAY				

Melting Points

mp °C	source
92.00	Alfa Aesar
94.00	PHYSPROP

N-(3-bromopropyl)phthalimide C11H10BrNO2[3, 64]

Compound Data



Melting point	**74.50 °C**	**347.65 K**			
CSID	20311	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	268.1066	**H bond donors**	0	**ACD/LogP**	2.85
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.58 g/cm^3
SMILES	O=C2c1ccccc1C(=O)N2CCCBr				

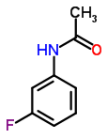
STD InChIKey	VKJCJJYNVIYVQR-UHFFFAOYAX

Melting Points

mp °C	source
74.00	Alfa Aesar
75.00	PHYSPROP

N-(3-fluorophenyl)acetamide C8H8FNO[3, 64]

Compound Data



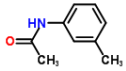
Melting point	**85.50 °C**	**358.65 K**			
CSID	9218	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	153.1536	**H bond donors**	1	**ACD/LogP**	1.61
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	O=C(Nc1cccc(F)c1)C				
STD InChIKey	AQLLDCFUQXGLHM-UHFFFAOYAE				

Melting Points

mp °C	source
88.00	Alfa Aesar
83.00	PHYSPROP

N-(3-methylphenyl)acetamide C9H11NO[61, 64]

Compound Data



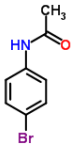
Melting point	**65.25 °C**	**338.40 K**			
CSID	11332993	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	149.1897	**H bond donors**	1	**ACD/LogP**	1.54
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	Cc1cccc(NC(C)=O)c1				
STD InChIKey	ALMHSXDYCFOZQD-UHFFFAOYAI				

Melting Points

mp °C	source
65.00	Oxford University MSDS
65.50	PHYSPROP

N-(4-bromophenyl)acetamide C8H8BrNO[2, 3, 64]

Compound Data



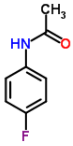
Melting point	**167.67 °C**	**440.82 K**			
CSID	7399	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	214.0592	**H bond donors**	1	**ACD/LogP**	2.29
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.54 g/cm^3
SMILES	Brc1ccc(NC(=O)C)cc1				
STD InChIKey	MSLICLMCQYQNPK-UHFFFAOYAL				

Melting Points

mp °C	source
166.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
169.00	Alfa Aesar
168.00	PHYSPROP

N-(4-fluorophenyl)acetanilide C8H8FNO[3, 64]

Compound Data



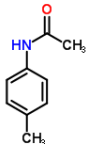
Melting point	**153.00 °C**	**426.15 K**			
CSID	9225	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	153.1536	**H bond donors**	1	**ACD/LogP**	1.47
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	O=C(Nc1ccc(F)cc1)C				
STD InChIKey	JHEFOJNPLXSWNZ-UHFFFAOYAX				

Melting Points

mp °C	source
152.00	Alfa Aesar
154.00	PHYSPROP

N-(4-methylphenyl)acetamide C9H11NO[3, 64]

Compound Data



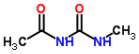
Melting point	**150.50 °C**	**423.65 K**			
CSID	10243171	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	149.1897	**H bond donors**	1	**ACD/LogP**	1.54
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	Cc1ccc(NC(C)=O)cc1				
STD InChIKey	YICAMJWHIUMFDI-UHFFFAOYAN				

Melting Points

mp °C	source
149.00	Alfa Aesar
152.00	PHYSPROP

N-(methylcarbamoyl)acetamid C4H8N2O2[48, 64]

Compound Data



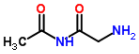
Melting point	**179.25 °C**	**452.40 K**			
CSID	62546	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	116.1185	**H bond donors**	2	**ACD/LogP**	-0.62
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.09 g/cm^3
SMILES	O=C(NC(=O)NC)C				
STD InChIKey	XRVHSOXXNQTWAW-UHFFFAOYAT				

Melting Points

mp °C	source
178.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
180.50	PHYSPROP

N-acetylglycinamide C4H8N2O2[3, 64]

Compound Data



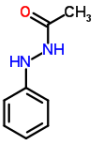
Melting point	**139.75 °C**	**412.90 K**			
CSID	68309	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	116.1185	**H bond donors**	3	**ACD/LogP**	-2.35
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	O=C(NC(=O)CN)C				
STD InChIKey	UUBCNZXOFCAIOX-UHFFFAOYAB				

Melting Points

mp °C	source
138.00	Alfa Aesar
141.50	PHYSPROP

N-acetylhydrazobenzene C8H10N2O[3, 64]

Compound Data



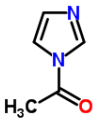
Melting point	**129.75 °C**	**402.90 K**			
CSID	7951	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1778	**H bond donors**	2	**ACD/LogP**	0.84
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C(NNc1ccccc1)C				
STD InChIKey	UICBCXONCUFSOI-UHFFFAOYAT				

Melting Points

mp °C	source

130.00	Alfa Aesar
129.50	PHYSPROP

N-acetylimidazole C5H6N2O[3, 64]



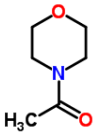
Compound Data

Melting point	**101.50 °C**	**374.65 K**			
CSID	16257	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	110.1139	**H bond donors**	0	**ACD/LogP**	-0.34
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.14 g/cm^3
SMILES	O=C(n1ccnc1)C				
STD InChIKey	VIHYIVKEECZGOU-UHFFFAOYAL				

Melting Points

mp °C	source
101.00	Alfa Aesar
102.00	PHYSPROP

N-acetylmorpholine C6H11NO2[3, 64]



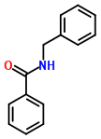
Compound Data

Melting point	**12.25 °C**	**285.40 K**			
CSID	14787	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	129.157	**H bond donors**	0	**ACD/LogP**	-0.32
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	O=C(N1CCOCC1)C				
STD InChIKey	KYWXRBNOYGGPIZ-UHFFFAOYAL				

Melting Points

mp °C	source
10.00	Alfa Aesar
14.50	PHYSPROP

N-benzylbenzamide C14H13NO[3, 48]



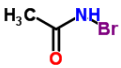
Compound Data

Melting point	**105.50 °C**	**378.65 K**			
CSID	66512	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	211.2591	**H bond donors**	1	**ACD/LogP**	2.95
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3
SMILES	O=C(NCc1ccccc1)c2ccccc2				
STD InChIKey	LKQUCICFTHBFAL-UHFFFAOYAQ				

Melting Points

mp °C	source
106.00	Alfa Aesar
105.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

n-bromoacetamide C2H4BrNO[3, 64]



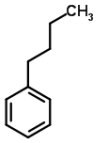
Compound Data

Melting point	**103.75 °C**	**376.90 K**			
CSID	4200	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	137.9633	**H bond donors**	1	**ACD/LogP**	0.44
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.71 g/cm^3
SMILES	BrNC(=O)C				
STD InChIKey	VBTQNRFWXBXZQR-UHFFFAOYAA				

Melting Points

mp °C	source
104.00	Alfa Aesar
103.50	PHYSPROP

n-butylbenzene C10H14[3, 4, 32, 61, 64]



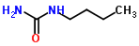
Compound Data

Melting point	**-87.96 °C**	**185.19 K**			
CSID	7419	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	4.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.86 g/cm^3
SMILES	c1ccccc1CCCC				
STD InChIKey	OCKPCBLVNKHBMX-UHFFFAOYAJ				

Melting Points

mp °C	source
-88.00	Alfa Aesar
-88.00	American Petroleum Institute. Research Project 44; Selected ...
-87.90	DrugBank
-88.00	Oxford University MSDS
-87.90	PHYSPROP

N-butylurea C5H12N2O[3, 64]



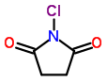
Compound Data

Melting point	**96.00 °C**	**369.15 K**			
CSID	11107	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	116.1616	**H bond donors**	3	**ACD/LogP**	0.37
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.96 g/cm^3
SMILES	O=C(N)NCCCC				
STD InChIKey	CNWSQCLBDWYLAN-UHFFFAOYAX				

Melting Points

mp °C	source
95.00	Alfa Aesar
97.00	PHYSPROP

N-chlorosuccinimide C4H4ClNO2[3, 64]



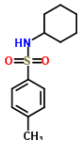
Compound Data

Melting point	**149.00 °C**	**422.15 K**			
CSID	29129	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	133.5331	**H bond donors**	0	**ACD/LogP**	-0.87
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.50 g/cm^3
SMILES	O=C1N(Cl)C(=O)CC1				
STD InChIKey	JRNVZBWKYDBUCA-UHFFFAOYAN				

Melting Points

mp °C	source
148.00	Alfa Aesar
150.00	PHYSPROP

N-cyclohexyl-4-methylbenzenesulfonamide C13H19NO2S[3, 61]



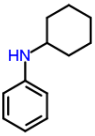
Compound Data

Melting point	**86.25 °C**	**359.40 K**			
CSID	6381	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	253.3605	**H bond donors**	1	**ACD/LogP**	3.49
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	O=S(=O)(NC1CCCCC1)c2ccc(cc2)C				
STD InChIKey	DKYVVNLWACXMDW-UHFFFAOYAU				

Melting Points

mp °C	source
88.00	Alfa Aesar
84.50	Oxford University MSDS

N-cyclohexylaniline C12H17N[3, 64]



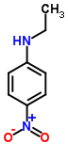
Compound Data

Melting point	**15.50 °C**	**288.65 K**			
CSID	67145	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	175.2701	**H bond donors**	1	**ACD/LogP**	3.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.02 g/cm^3
SMILES	c2c(NC1CCCCC1)cccc2				
STD InChIKey	TXTHKGMZDDTZFD-UHFFFAOYAU				

Melting Points

mp °C	source
15.00	Alfa Aesar
16.00	PHYSPROP

N-ethyl-4-nitroaniline C8H10N2O2[61, 64]



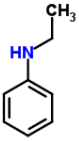
Compound Data

Melting point	**96.50 °C**	**369.65 K**			
CSID	18227	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	166.1772	**H bond donors**	1	**ACD/LogP**	2.57
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.21 g/cm^3
SMILES	[O-][N+](=O)c1ccc(NCC)cc1				
STD InChIKey	XBNNLAWQCMDISJ-UHFFFAOYAU				

Melting Points

mp °C	source
96.00	Oxford University MSDS
97.00	PHYSPROP

N-ethylaniline C8H11N[2, 3, 61, 64]



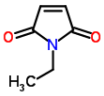
Compound Data

Melting point	**-63.62 °C**	**209.52 K**			
CSID	7387	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	1	**ACD/LogP**	2.13
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	N(c1ccccc1)CC				
STD InChIKey	OJGMBLNIHDZDGS-UHFFFAOYAD				

Melting Points

mp °C	source
-63.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-64.00	Alfa Aesar
-64.00	Oxford University MSDS
-63.50	PHYSPROP

N-ethylmaleimide C6H7NO2[3, 61, 64]



Compound Data

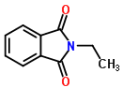
Melting point	**44.83 °C**	**317.98 K**			
CSID	4209	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	125.1253	**H bond donors**	0	**ACD/LogP**	0.68
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	O=C1\C=C/C(=O)N1CC				
STD InChIKey	HDFGOPSGAURCEO-UHFFFAOYAE				

Melting Points

mp °C	source
45.00	Alfa Aesar
44.00	Oxford University MSDS

45.50	PHYSPROP

N-ethylphthalimide C10H9NO2[3, 64]



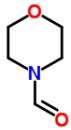
Compound Data

Melting point	**77.50 °C**	**350.65 K**			
CSID	19862	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	175.184	**H bond donors**	0	**ACD/LogP**	2.09
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	O=C2c1ccccc1C(=O)N2CC				
STD InChIKey	JZDSOQSUCWVBMV-UHFFFAOYAZ				

Melting Points

mp °C	source
76.00	Alfa Aesar
79.00	PHYSPROP

N-formylmorpholine C5H9NO2[3, 64]



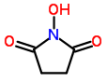
Compound Data

Melting point	**21.50 °C**	**294.65 K**			
CSID	19231	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	115.1305	**H bond donors**	0	**ACD/LogP**	-1.30
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.21 g/cm^3
SMILES	O=CN1CCOCC1				
STD InChIKey	LCEDQNDDFOCWGG-UHFFFAOYAJ				

Melting Points

mp °C	source
22.00	Alfa Aesar
21.00	PHYSPROP

N-hydroxysuccinimide C4H5NO3[3, 61]



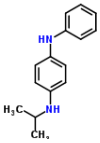
Compound Data

Melting point	**96.75 °C**	**369.90 K**			
CSID	72416	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	115.0874	**H bond donors**	1	**ACD/LogP**	-2.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.65 g/cm^3
SMILES	O=C1N(O)C(=O)CC1				
STD InChIKey	NQTADLQHYWFPDB-UHFFFAOYAM				

Melting Points

mp °C	source
97.00	Alfa Aesar
96.50	Oxford University MSDS

N-isopropyl-N'-phenyl-p-phenylenediamine C15H18N2[3, 64]



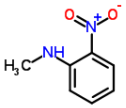
Compound Data

Melting point	**75.50 °C**	**348.65 K**			
CSID	7292	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	226.3168	**H bond donors**	2	**ACD/LogP**	2.83
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	N(c1ccc(cc1)Nc2ccccc2)C(C)C				
STD InChIKey	OUBMGJOQLXMSNT-UHFFFAOYAN				

Melting Points

mp °C	source
77.00	Alfa Aesar
74.00	PHYSPROP

N-methyl-2-nitroaniline C7H8N2O2[3, 64]



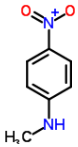
Compound Data

Melting point	**36.50 °C**	**309.65 K**			
CSID	62372	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	1	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.26 g/cm^3
SMILES	[O-][N+](=O)c1ccccc1NC				
STD InChIKey	KFBOUJZFFJDYTA-UHFFFAOYAI				

Melting Points

mp °C	source
35.00	Alfa Aesar
38.00	PHYSPROP

N-methyl-4-nitroaniline C7H8N2O2[3, 61, 64]



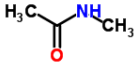
Compound Data

Melting point	**152.33 °C**	**425.48 K**			
CSID	7203	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	152.1506	**H bond donors**	1	**ACD/LogP**	2.04
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.26 g/cm^3
SMILES	[O-][N+](=O)c1ccc(NC)cc1				
STD InChIKey	XIFJZJPMHNUGRA-UHFFFAOYAM				

Melting Points

mp °C	source
153.00	Alfa Aesar
152.00	Oxford University MSDS
152.00	PHYSPROP

N-methylacetamide C3H7NO[3, 61, 64]



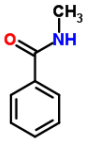
Compound Data

Melting point	**27.33 °C**	**300.48 K**			
CSID	6334	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	73.0938	**H bond donors**	1	**ACD/LogP**	-1.05
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	O=C(NC)C				
STD InChIKey	OHLUUHNLEMFGTQ-UHFFFAOYAK				

Melting Points

mp °C	source
27.00	Alfa Aesar
27.00	Oxford University MSDS
28.00	PHYSPROP

N-methylbenzamide C8H9NO[3, 64]



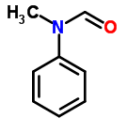
Compound Data

Melting point	**80.50 °C**	**353.65 K**			
CSID	11460	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	1	**ACD/LogP**	0.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	O=C(NC)c1ccccc1				
STD InChIKey	NCCHARWOCKOHIH-UHFFFAOYAK				

Melting Points

mp °C	source
79.00	Alfa Aesar
82.00	PHYSPROP

N-methylformanilide C8H9NO[3, 64]



Compound Data

Melting point	**12.75 °C**	**285.90 K**			
CSID	60103	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	135.1632	**H bond donors**	0	**ACD/LogP**	1.09
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.08 g/cm^3
SMILES	O=CN(c1ccccc1)C				
STD InChIKey	JIKUXBYRTXDNIY-UHFFFAOYAF				

Melting Points

mp °C	source
11.00	Alfa Aesar
14.50	PHYSPROP

N-methylsuccinimide C5H7NO2[3, 64]

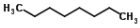
Compound Data

Melting point	**68.50 °C**	**341.65 K**			
CSID	63882	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	113.1146	**H bond donors**	0	**ACD/LogP**	-0.95
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.22 g/cm^3
SMILES	O=C1N(C(=O)CC1)C				
STD InChIKey	KYEACNNYFNZCST-UHFFFAOYAZ				

Melting Points

mp °C	source
66.00	Alfa Aesar
71.00	PHYSPROP

n-octane C8H18[3, 4, 32, 59, 64]



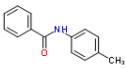
Compound Data

Melting point	**-56.89 °C**	**216.26 K**			
CSID	349	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	114.2285	**H bond donors**	0	**ACD/LogP**	5.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.71 g/cm^3
SMILES	CCCCCCCC				
STD InChIKey	TVMXDCGIABBOFY-UHFFFAOYAY				

Melting Points

mp °C	source
-57.00	Alfa Aesar
-57.00	American Petroleum Institute. Research Project 44; Selected ...
-56.80	DrugBank
-56.85	NIST Web Book
-56.80	PHYSPROP

N-p-tolyl-benzamide C14H13NO[48, 64]



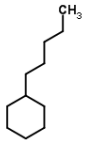
Compound Data

Melting point	**157.00 °C**	**430.15 K**			
CSID	10274392	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	211.2591	**H bond donors**	1	**ACD/LogP**	3.35
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.15 g/cm^3
SMILES	Cc1ccc(cc1)NC(=O)c2ccccc2				
STD InChIKey	YUIHXKGKVSVIEL-UHFFFAOYAA				

Melting Points

mp °C	source
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
158.00	PHYSPROP

n-pentylcyclohexane C11H22[3, 4, 64]



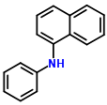
Compound Data

Melting point	**-57.83 °C**	**215.32 K**			
CSID	19110	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	154.2924	**H bond donors**	0	**ACD/LogP**	6.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.80 g/cm^3
SMILES	C(CCC1CCCCC1)CC				
STD InChIKey	HLTMUYBTNSVOFY-UHFFFAOYAD				

Melting Points

mp °C	source
-58.00	Alfa Aesar
-58.00	American Petroleum Institute. Research Project 44; Selected ...
-57.50	PHYSPROP

N-phenyl-1-naphthaleneamine C16H13N[61, 64]



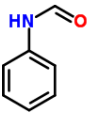
Compound Data

Melting point	**61.50 °C**	**334.65 K**			
CSID	6746	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	219.2811	**H bond donors**	1	**ACD/LogP**	4.20
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.16 g/cm^3
SMILES	c3c(Nc1ccccc1)c2ccccc2cc3				
STD InChIKey	XQVWYOYUZDUNRW-UHFFFAOYAN				

Melting Points

mp °C	source
61.00	Oxford University MSDS
62.00	PHYSPROP

N-phenylformamide C7H7NO[3, 61, 64]



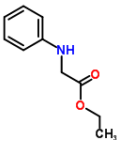
Compound Data

Melting point	**46.67 °C**	**319.82 K**			
CSID	7388	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	121.1366	**H bond donors**	1	**ACD/LogP**	1.15
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	O=CNc1ccccc1				
STD InChIKey	DYDNPESBYVVLBO-UHFFFAOYAU				

Melting Points

mp °C	source
47.00	Alfa Aesar
47.00	Oxford University MSDS
46.00	PHYSPROP

N-phenylglycine ethyl ester C10H13NO2[3, 64]



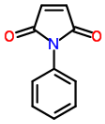
Compound Data

Melting point	**57.50 °C**	**330.65 K**			
CSID	21159611	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	179.2157	**H bond donors**	1	**ACD/LogP**	1.79
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.11 g/cm^3
SMILES	CCOC(=O)CNc1ccccc1				
STD InChIKey	MLSGRWDEDYJNER-UHFFFAOYAC				

Melting Points

mp °C	source
57.00	Alfa Aesar
58.00	PHYSPROP

N-phenylmaleimide C10H7NO2[3, 64]



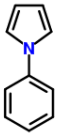
Compound Data

Melting point	**89.75 °C**	**362.90 K**			
CSID	13073	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	173.1681	**H bond donors**	0	**ACD/LogP**	1.15
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.33 g/cm^3
SMILES	c1ccc(cc1)N2C(=O)C=CC2=O				
STD InChIKey	HIDBROSJWZYGSZ-UHFFFAOYAO				

Melting Points

mp °C	source
89.00	Alfa Aesar
90.50	PHYSPROP

N-phenylpyrrole C10H9N[3, 64]



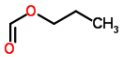
Compound Data

Melting point	**60.50 °C**	**333.65 K**			
CSID	11970	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	0	**ACD/LogP**	3.08
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.97 g/cm^3
SMILES	c1ccc(cc1)n2cccc2				
STD InChIKey	GEZGAZKEOUKLBR-UHFFFAOYAM				

Melting Points

mp °C	source
59.00	Alfa Aesar
62.00	PHYSPROP

n-propyl formate C4H8O2[3, 64]



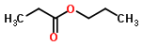
Compound Data

Melting point	**-92.95 °C**	**180.20 K**			
CSID	7782	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1051	**H bond donors**	0	**ACD/LogP**	0.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.90 g/cm^3
SMILES	O=COCCC				
STD InChIKey	KFNNIILCVOLYIR-UHFFFAOYAC				

Melting Points

mp °C	source
-93.00	Alfa Aesar
-92.90	PHYSPROP

n-propyl propionate C6H12O2[3, 64]



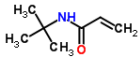
Compound Data

Melting point	**-75.95 °C**	**197.20 K**			
CSID	7515	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	116.1583	**H bond donors**	0	**ACD/LogP**	1.77
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.89 g/cm^3
SMILES	O=C(OCCC)CC				
STD InChIKey	MCSINKKTEDDPNK-UHFFFAOYAX				

Melting Points

mp °C	source
-76.00	Alfa Aesar
-75.90	PHYSPROP

N-t-butylacrylamide C7H13NO[3, 64]



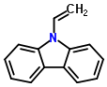
Compound Data

Melting point	**128.75 °C**	**401.90 K**			
CSID	7589	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	127.1842	**H bond donors**	1	**ACD/LogP**	0.55
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.88 g/cm^3
SMILES	O=C(\C=C)NC(C)(C)C				
STD InChIKey	XFHJDMUEHUHAJW-UHFFFAOYAL				

Melting Points

mp °C	source
129.00	Alfa Aesar
128.50	PHYSPROP

N-vinylcarbazole C14H11N[61, 64]



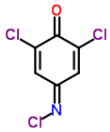
Compound Data

Melting point	**64.00 °C**	**337.15 K**			
CSID	14414	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	193.2438	**H bond donors**	0	**ACD/LogP**	4.61
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.05 g/cm^3
SMILES	c1cccc3c1c2c(cccc2)n3\C=C				
STD InChIKey	KKFHAJHLJHVUDM-UHFFFAOYAO				

Melting Points

mp °C	source
63.00	Oxford University MSDS
65.00	PHYSPROP

N,2,6-trichloroquinoneimine C6H2Cl3NO[61, 64]



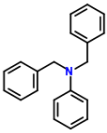
Compound Data

Melting point	**66.50 °C**	**339.65 K**			
CSID	7275	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	210.4452	**H bond donors**	0	**ACD/LogP**	1.64
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.61 g/cm^3
SMILES	Cl\C1=CC(=N\Cl)/C=C(/Cl)C1=O				
STD InChIKey	YHUMTHWQGWPJOQ-UHFFFAOYAO				

Melting Points

mp °C	source
67.00	Oxford University MSDS
66.00	PHYSPROP

N,N-dibenzylaniline C20H19N[3, 64]



Compound Data

Melting point	**69.50 °C**	**342.65 K**			
CSID	60047	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	273.3716	**H bond donors**	0	**ACD/LogP**	6.06
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.10 g/cm^3
SMILES	c1(ccccc1)CN(c2ccccc2)Cc3ccccc3				
STD InChIKey	ISGXOWLMGOPVPB-UHFFFAOYAN				

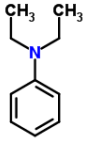
Melting Points

mp °C	source
70.00	Alfa Aesar
69.00	PHYSPROP

N,N-diethylaniline C10H15N[2, 3, 61, 64]

Compound Data

Melting point	**-38.20 °C**	**234.95 K**	



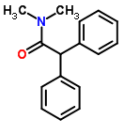
CSID	6794	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	149.2328	**H bond donors**	0	**ACD/LogP**	3.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.93 g/cm^3
SMILES	N(c1ccccc1)(CC)CC				
STD InChIKey	GGSUCNLOZRCGPQ-UHFFFAOYAA				

Melting Points

mp °C	source
-38.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-38.00	Alfa Aesar
-38.00	Oxford University MSDS
-38.80	PHYSPROP

N,N-dimethyl-2,2-diphenylacetamide C16H17NO[61, 64]

Compound Data



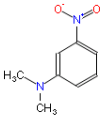
Melting point	**134.25 °C**	**407.40 K**			
CSID	13133	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	239.3123	**H bond donors**	0	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	O=C(N(C)C)C(c1ccccc1)c2ccccc2				
STD InChIKey	QAHFOPIILNICLA-UHFFFAOYAX				

Melting Points

mp °C	source
133.50	Oxford University MSDS
135.00	PHYSPROP

N,N-dimethyl-3-nitroaniline C8H10N2O2[3, 64]

Compound Data



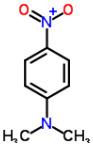
Melting point	**59.75 °C**	**332.90 K**			
CSID	21168823	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	166.1772	**H bond donors**	0	**ACD/LogP**	2.74
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	CN(C)c1cccc(c1)[N+](=O)[O-]				
STD InChIKey	CJDICMLSLYHRPT-UHFFFAOYAB				

Melting Points

mp °C	source
59.00	Alfa Aesar
60.50	PHYSPROP

N,N-dimethyl-4-nitroaniline C8H10N2O2[3, 64]

Compound Data



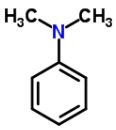
Melting point	**164.50 °C**	**437.65 K**			
CSID	7210	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	166.1772	**H bond donors**	0	**ACD/LogP**	2.61
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	[O-][N+](=O)c1ccc(N(C)C)cc1				
STD InChIKey	QJAIOCKFIORVFU-UHFFFAOYAA				

Melting Points

mp °C	source
165.00	Alfa Aesar
164.00	PHYSPROP

N,N-dimethylaniline C8H11N[2, 3, 61, 64]

Compound Data



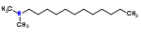
Melting point	**2.38 °C**	**275.52 K**			
CSID	924	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	121.1796	**H bond donors**	0	**ACD/LogP**	2.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.95 g/cm^3
SMILES	N(c1ccccc1)(C)C				
STD InChIKey	JLTDJTHDQAWBAV-UHFFFAOYAJ				

Melting Points

mp °C	source
3.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
2.00	Alfa Aesar
2.00	Oxford University MSDS
2.50	PHYSPROP

N,N-dimethyldodecylamine C14H31N[3, 64]

Compound Data



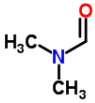
Melting point	**-17.50 °C**	**255.65 K**			
CSID	7876	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	213.4026	**H bond donors**	0	**ACD/LogP**	5.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.80 g/cm^3
SMILES	N(CCCCCCCCCCCC)(C)C				
STD InChIKey	YWFWDNVOPHGWMX-UHFFFAOYAY				

Melting Points

mp °C	source
-20.00	Alfa Aesar
-15.00	PHYSPROP

N,N-dimethylformamide C3H7NO[2, 3, 32, 61, 64]

Compound Data



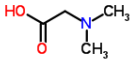
Melting point	**-60.76 °C**	**212.39 K**			
CSID	5993	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	73.0938	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.89 g/cm^3
SMILES	CN(C)C=O				
STD InChIKey	ZMXDDKWLCZADIW-UHFFFAOYAS				

Melting Points

mp °C	source
-61.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-61.00	Alfa Aesar
-60.40	DrugBank
-61.00	Oxford University MSDS
-60.40	PHYSPROP

N,N-dimethylglycine C4H9NO2[3, 32, 64]

Compound Data



Melting point	**184.00 °C**	**457.15 K**			
CSID	653	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	103.1198	**H bond donors**	1	**ACD/LogP**	-0.30
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.07 g/cm^3
SMILES	O=C(O)CN(C)C				
STD InChIKey	FFDGPVCHZBVARC-UHFFFAOYAX				

Melting Points

mp °C	source
181.00	Alfa Aesar
185.50	DrugBank
185.50	PHYSPROP

N,N-dimethylurea C3H8N2O[3, 64]

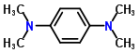
Compound Data

Melting point	**181.75 °C**	**454.90 K**			
CSID	11244	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	88.1084	**H bond donors**	2	**ACD/LogP**	-1.28
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.02 g/cm^3
SMILES	O=C(N)N(C)C				
STD InChIKey	YBBLOADPFWKNGS-UHFFFAOYAG				

Melting Points

mp °C	source
180.00	Alfa Aesar
183.50	PHYSPROP

N,N,N',N'-tetramethyl-p-phenylenediamine C10H16N2[3, 64]



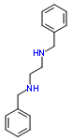
Compound Data

Melting point	**50.50 °C**	**323.65 K**			
CSID	21106585	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	164.2474	**H bond donors**	0	**ACD/LogP**	2.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	CN(C)c1ccc(cc1)N(C)C				
STD InChIKey	CJAOGUFAAWZWNI-UHFFFAOYAJ				

Melting Points

mp °C	source
50.00	Alfa Aesar
51.00	PHYSPROP

N,N'-dibenzylethylenediamine C16H20N2[3, 64]



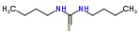
Compound Data

Melting point	**25.00 °C**	**298.15 K**			
CSID	8463	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	240.3434	**H bond donors**	2	**ACD/LogP**	2.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	1.03 g/cm^3
SMILES	N(CCNCc1ccccc1)Cc2ccccc2				
STD InChIKey	JUHORIMYRDESRB-UHFFFAOYAS				

Melting Points

mp °C	source
24.00	Alfa Aesar
26.00	PHYSPROP

N,N'-dibutylthiourea C9H20N2S[3, 64]



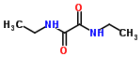
Compound Data

Melting point	**65.00 °C**	**338.15 K**			
CSID	2005824	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	188.3335	**H bond donors**	2	**ACD/LogP**	2.84
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	0.94 g/cm^3
SMILES	S=C(NCCCC)NCCCC				
STD InChIKey	KFFQABQEJATQAT-UHFFFAOYAB				

Melting Points

mp °C	source
66.00	Alfa Aesar
64.00	PHYSPROP

N,N'-diethyloxamide C6H12N2O2[3, 64]



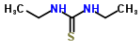
Compound Data

Melting point	**177.50 °C**	**450.65 K**			
CSID	62423	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	144.1717	**H bond donors**	2	**ACD/LogP**	-0.23
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.03 g/cm^3
SMILES	O=C(NCC)C(=O)NCC				
STD InChIKey	FFYAVOJIYAAUNX-UHFFFAOYAN				

Melting Points

mp °C	source
180.00	Alfa Aesar
175.00	PHYSPROP

N,N'-diethylthiourea C5H12N2S[3, 64]



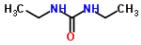
Compound Data

Melting point	**77.50 °C**	**350.65 K**			
CSID	2016737	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	132.2272	**H bond donors**	2	**ACD/LogP**	0.72
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.99 g/cm^3
SMILES	S=C(NCC)NCC				
STD InChIKey	FLVIGYVXZHLUHP-UHFFFAOYAN				

Melting Points

mp °C	source
77.00	Alfa Aesar
78.00	PHYSPROP

N,N'-diethylurea C5H12N2O[3, 64]



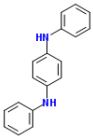
Compound Data

Melting point	**111.25 °C**	**384.40 K**			
CSID	11694	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	116.1616	**H bond donors**	2	**ACD/LogP**	0.05
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.92 g/cm^3
SMILES	O=C(NCC)NCC				
STD InChIKey	ZWAVGZYKJNOTPX-UHFFFAOYAT				

Melting Points

mp °C	source
110.00	Alfa Aesar
112.50	PHYSPROP

N,N'-diphenyl-p-phenylenediamine C18H16N2[3, 64]



Compound Data

Melting point	**145.50 °C**	**418.65 K**			
CSID	6080	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	260.333	**H bond donors**	2	**ACD/LogP**	4.54
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	c1ccc(cc1)Nc2ccc(cc2)Nc3ccccc3				
STD InChIKey	UTGQNNCQYDRXCH-UHFFFAOYAQ				

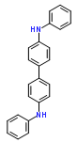
Melting Points

mp °C	source
147.00	Alfa Aesar
144.00	PHYSPROP

N,N'-diphenylbenzidine C24H20N2[3, 64]

Compound Data

Melting point	**247.50 °C**	**520.65 K**



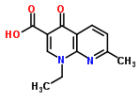
CSID	61577	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	336.429	**H bond donors**	2	**ACD/LogP**	6.34
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.17 g/cm^3
SMILES	c4c(Nc1ccc(cc1)c3ccc(Nc2ccccc2)cc3)cccc4				
STD InChIKey	FDRNXKXKFNHNCA-UHFFFAOYAV				

Melting Points

mp °C	source
248.00	Alfa Aesar
247.00	PHYSPROP

nalidixic acid C12H12N2O3[3, 32, 44, 61, 64]

Compound Data



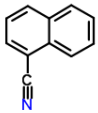
Melting point	**229.40 °C**	**502.55 K**			
CSID	4268	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	232.2353	**H bond donors**	1	**ACD/LogP**	1.19
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=C\2c1c(nc(cc1)C)N(/C=C/2C(=O)O)CC				
STD InChIKey	MHWLWQUZZRMNGJ-UHFFFAOYAS				

Melting Points

mp °C	source
229.00	Alfa Aesar
229.50	DrugBank
229.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
229.50	Oxford University MSDS
229.50	PHYSPROP

naphthalene-1-carbonitrile C11H7N[3, 64]

Compound Data



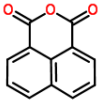
Melting point	**36.75 °C**	**309.90 K**			
CSID	6585	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	153.18	**H bond donors**	0	**ACD/LogP**	2.89
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	N#Cc2cccc1ccccc12				
STD InChIKey	YJMNOKOLADGBKA-UHFFFAOYAU				

Melting Points

mp °C	source
36.00	Alfa Aesar
37.50	PHYSPROP

naphthalic anhydride C12H6O3[3, 64]

Compound Data

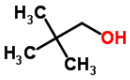


Melting point	**270.50 °C**	**543.65 K**			
CSID	6438	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	198.1742	**H bond donors**	0	**ACD/LogP**	1.75
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.45 g/cm^3
SMILES	O=C3OC(=O)c2cccc1cccc3c12				
STD InChIKey	GRSMWKLPSNHDHA-UHFFFAOYAM				

Melting Points

mp °C	source
271.00	Alfa Aesar
270.00	PHYSPROP

neopentyl alcohol C5H12O[3, 4, 64]



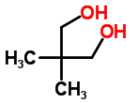
Compound Data

Melting point	**52.17 °C**	**325.32 K**			
CSID	6164	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	88.1482	**H bond donors**	1	**ACD/LogP**	1.04
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.81 g/cm^3
SMILES	OCC(C)(C)C				
STD InChIKey	KPSSIOMAKSHJJG-UHFFFAOYAJ				

Melting Points

mp °C	source
54.00	Alfa Aesar
50.00	American Petroleum Institute. Research Project 44; Selected ...
52.50	PHYSPROP

neopentyl glycol C5H12O2[2, 3, 61, 64]



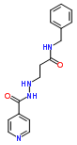
Compound Data

Melting point	**127.25 °C**	**400.40 K**			
CSID	13835293	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	104.1476	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	0.98 g/cm^3
SMILES	CC(C)(CO)CO				
STD InChIKey	SLCVBVWXLSEKPL-UHFFFAOYAD				

Melting Points

mp °C	source
126.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
128.00	Alfa Aesar
125.00	Oxford University MSDS
130.00	PHYSPROP

nialamide C16H18N4O2[32, 64]



Compound Data

Melting point	**151.30 °C**	**424.45 K**			
CSID	4317	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	298.3397	**H bond donors**	3	**ACD/LogP**	0.32
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.20 g/cm^3
SMILES	O=C(NNCCC(=O)NCc1ccccc1)c2ccncc2				
STD InChIKey	NOIIUHRQUVNIDD-UHFFFAOYAU				

Melting Points

mp °C	source
151.60	DrugBank
151.00	PHYSPROP

nicotinamide C6H6N2O[3, 32, 44, 61, 64]

Compound Data

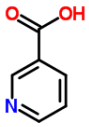
Melting point	**129.90 °C**	**403.05 K**			
CSID	911	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	122.1246	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.21 g/cm^3
SMILES	c1cc(cnc1)C(=O)N				
STD InChIKey	DFPAKSUCGFBDDF-UHFFFAOYAZ				

Melting Points

mp °C	source
130.00	Alfa Aesar
130.00	DrugBank
129.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
130.00	Oxford University MSDS

130.00	PHYSPROP

nicotinic acid C6H5NO2[3, 32, 35, 44, 61, 64]



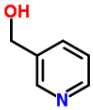
Compound Data

Melting point	**236.97 °C**	**510.12 K**			
CSID	913	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	123.1094	**H bond donors**	1	**ACD/LogP**	0.22
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	c1cc(cnc1)C(=O)O				
STD InChIKey	PVNIIMVLHYAWGP-UHFFFAOYAA				

Melting Points

mp °C	source
238.00	Alfa Aesar
237.00	DrugBank
236.60	EPISuite-ChemSpider
236.60	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
237.00	Oxford University MSDS
236.60	PHYSPROP

nicotinyl alcohol C6H7NO[3, 64]



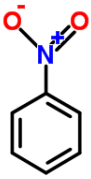
Compound Data

Melting point	**-6.75 °C**	**266.40 K**			
CSID	7229	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	109.1259	**H bond donors**	1	**ACD/LogP**	-0.46
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.13 g/cm^3
SMILES	OCc1cccnc1				
STD InChIKey	MVQVNTPHUGQQHK-UHFFFAOYAK				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-6.50	PHYSPROP

nitrobenzene C6H5NO2[2, 3, 61, 64]



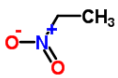
Compound Data

Melting point	**5.67 °C**	**278.82 K**			
CSID	7138	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	123.1094	**H bond donors**	0	**ACD/LogP**	1.92
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	c1ccc(cc1)[N+](=O)[O-]				
STD InChIKey	LQNUZADURLCDLV-UHFFFAOYAA				

Melting Points

mp °C	source
6.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
6.00	Alfa Aesar
5.00	Oxford University MSDS
5.70	PHYSPROP

nitroethane C2H5NO2[3, 64]



Compound Data

Melting point	**-89.25 °C**	**183.90 K**			
CSID	6338	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	75.07	**H bond donors**	0	**ACD/LogP**	0.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.01 g/cm^3
SMILES	CC[N+](=O)[O-]				

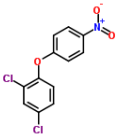
STD InChIKey	MCSAJNNLRCFZED-UHFFFAOYAB

Melting Points

mp °C	source
-89.00	Alfa Aesar
-89.50	PHYSPROP

nitrofen C12H7Cl2NO3[3, 61, 64]

Compound Data



Melting point	**70.17 °C**	**343.32 K**			
CSID	15010	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	284.0949	**H bond donors**	0	**ACD/LogP**	4.92
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.45 g/cm^3
SMILES	Clc2cc(Cl)ccc2Oc1ccc([N+]([O-])=O)cc1				
STD InChIKey	XITQUSLLOSKDTB-UHFFFAOYAU				

Melting Points

mp °C	source
70.00	Alfa Aesar
70.50	Oxford University MSDS
70.00	PHYSPROP

nitromethane CH3NO2[3, 61, 64]

Compound Data

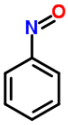
Melting point	**-28.83 °C**	**244.32 K**			
CSID	6135	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	61.04	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	C[N+](=O)[O-]				
STD InChIKey	LYGJENNIWJXYER-UHFFFAOYAW				

Melting Points

mp °C	source
-29.00	Alfa Aesar
-29.00	Oxford University MSDS
-28.50	PHYSPROP

nitrosobenzene C6H5NO[61, 64]

Compound Data



Melting point	**66.75 °C**	**339.90 K**			
CSID	10989	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	107.11	**H bond donors**	0	**ACD/LogP**	2.01
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.04 g/cm^3
SMILES	O=Nc1ccccc1				
STD InChIKey	NLRKCXQQSUWLCH-UHFFFAOYAR				

Melting Points

mp °C	source
65.00	Oxford University MSDS
68.50	PHYSPROP

nonacosane C29H60[61, 64]

Compound Data

Melting point	**64.85 °C**	**338.00 K**			
CSID	11903	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	408.7867	**H bond donors**	0	**ACD/LogP**	16.16
Phase 25 °C	solid	**Rotatable bonds**	26	**Predicted density**	0.81 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCCC)CCCCCC				

STD InChIKey	IGGUPRCHHJZPBS-UHFFFAOYAH

Melting Points

mp °C	source
66.00	Oxford University MSDS
63.70	PHYSPROP

nonadecane C19H40[3, 4, 61, 64]

Compound Data

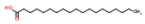
Melting point	**32.52 °C**	**305.67 K**			
CSID	11895	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	268.5209	**H bond donors**	0	**ACD/LogP**	10.39
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	0.79 g/cm^3
SMILES	CCCCCCCCCCCCCCCCCCCC				
STD InChIKey	LQERIDTXQFOHKA-UHFFFAOYAM				

Melting Points

mp °C	source
33.00	Alfa Aesar
32.00	American Petroleum Institute. Research Project 44; Selected ...
33.00	Oxford University MSDS
32.10	PHYSPROP

nonadecanoic acid C19H38O2[61, 64]

Compound Data



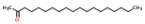
Melting point	**69.20 °C**	**342.35 K**			
CSID	12071	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	298.5038	**H bond donors**	1	**ACD/LogP**	8.75
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.89 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCCCCCC				
STD InChIKey	ISYWECDDZWTKFF-UHFFFAOYAR				

Melting Points

mp °C	source
69.00	Oxford University MSDS
69.40	PHYSPROP

nonadecanone C19H38O[3, 64]

Compound Data



Melting point	**56.00 °C**	**329.15 K**			
CSID	62631	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	282.5044	**H bond donors**	0	**ACD/LogP**	8.34
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	0.83 g/cm^3
SMILES	O=C(CCCCCCCCCCCCCCCCCC)C				
STD InChIKey	IEDKVDCIEARIIU-UHFFFAOYAV				

Melting Points

mp °C	source
55.00	Alfa Aesar
57.00	PHYSPROP

nonane C9H20[3, 4, 61, 64]

Compound Data

Melting point	**-53.38 °C**	**219.77 K**			
CSID	7849	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	128.2551	**H bond donors**	0	**ACD/LogP**	5.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.72 g/cm^3
SMILES	CCCCCCCCC				

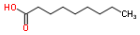
STD InChIKey	BKIMMITUMNQMOS-UHFFFAOYAS

Melting Points

mp °C	source
-53.00	Alfa Aesar
-54.00	American Petroleum Institute. Research Project 44; Selected ...
-53.00	Oxford University MSDS
-53.50	PHYSPROP

nonanoic acid C9H18O2[3, 4, 64]

Compound Data



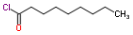
Melting point	**11.43 °C**	**284.58 K**			
CSID	7866	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.238	**H bond donors**	1	**ACD/LogP**	3.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.92 g/cm^3
SMILES	O=C(O)CCCCCCCC				
STD InChIKey	FBUKVWPVBMHYJY-UHFFFAOYAF				

Melting Points

mp °C	source
10.00	Alfa Aesar
12.00	American Petroleum Institute. Research Project 44; Selected ...
12.30	PHYSPROP

nonanoyl chloride C9H17ClO[3, 64]

Compound Data



Melting point	**-60.75 °C**	**212.40 K**			
CSID	63017	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	176.6837	**H bond donors**	0	**ACD/LogP**	4.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.95 g/cm^3
SMILES	ClC(=O)CCCCCCCC				
STD InChIKey	NTQYXUJLILNTFH-UHFFFAOYAD				

Melting Points

mp °C	source
-61.00	Alfa Aesar
-60.50	PHYSPROP

octacosane C28H58[3, 64]

Compound Data

Melting point	**63.25 °C**	**336.40 K**			
CSID	11902	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	394.7601	**H bond donors**	0	**ACD/LogP**	15.63
Phase 25 °C	solid	**Rotatable bonds**	25	**Predicted density**	0.80 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCC)CCCCCC				
STD InChIKey	ZYURHZPYMFLWSH-UHFFFAOYAH				

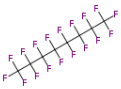
Melting Points

mp °C	source
62.00	Alfa Aesar
64.50	PHYSPROP

octadecafluorooctane C8F18[61, 64]

Compound Data

Melting point	**-24.10 °C**	**249.05 K**			
CSID	9018	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	438.0569	**H bond donors**	0	**ACD/LogP**	7.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	1.69 g/cm^3



SMILES	FC(F)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
STD InChIKey	YVBBRRALBYAZBM-UHFFFAOYAG

Melting Points

mp °C	source
-25.00	Oxford University MSDS
-23.20	PHYSPROP

octadecane C18H38[3, 4, 64]

Compound Data

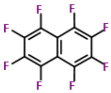
Melting point	**28.07 °C**	**301.22 K**			
CSID	11145	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	254.4943	**H bond donors**	0	**ACD/LogP**	10.32
Phase 25 °C	solid	**Rotatable bonds**	15	**Predicted density**	0.78 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCC)C				
STD InChIKey	RZJRJXONCZWCBN-UHFFFAOYAL				

Melting Points

mp °C	source
28.00	Alfa Aesar
28.00	American Petroleum Institute. Research Project 44; Selected ...
28.20	PHYSPROP

octafluoronaphthalene C10F8[3, 64]

Compound Data



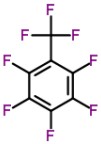
Melting point	**87.25 °C**	**360.40 K**			
CSID	60886	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	272.0942	**H bond donors**	0	**ACD/LogP**	3.61
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.73 g/cm^3
SMILES	Fc2c1c(F)c(F)c(F)c(F)c1c(F)c(F)c2F				
STD InChIKey	JDCMOHAFGDQQJX-UHFFFAOYAI				

Melting Points

mp °C	source
87.00	Alfa Aesar
87.50	PHYSPROP

octafluorotoluene C7F8[3, 64]

Compound Data



Melting point	**-65.80 °C**	**207.35 K**			
CSID	9522	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	236.0621	**H bond donors**	0	**ACD/LogP**	2.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.64 g/cm^3
SMILES	Fc1c(c(F)c(F)c(F)c1F)C(F)(F)F				
STD InChIKey	USPWUOFNOTUBAD-UHFFFAOYAB				

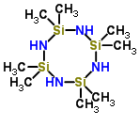
Melting Points

mp °C	source
-66.00	Alfa Aesar
-65.60	PHYSPROP

octamethylcyclotetrasilazane C8H28N4Si4[3, 64]

Compound Data

Melting point	**96.75 °C**	**369.90 K**			



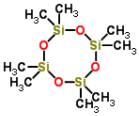
CSID	59489	**H bond acceptors**	4	**Rule of 5 violations**	NA
Molecular weight	292.6767	**H bond donors**	4	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.92 g/cm^3
SMILES	N1[Si](N[Si](N[Si]1(C)C)(C)C)(C)C)(C)C				
STD InChIKey	FIADVASZMLCQIF-UHFFFAOYAF				

Melting Points

mp °C	source
96.00	Alfa Aesar
97.50	PHYSPROP

octamethylcyclotetrasiloxane C8H24O4Si4[3, 61, 64]

Compound Data



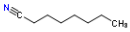
Melting point	**17.67 °C**	**290.82 K**			
CSID	10696	**H bond acceptors**	4	**Rule of 5 violations**	NA
Molecular weight	296.6158	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.95 g/cm^3
SMILES	O1[Si](O[Si](O[Si]1(C)C)(C)C)(C)C)(C)C				
STD InChIKey	HMMGMWAXVFQUOA-UHFFFAOYAZ				

Melting Points

mp °C	source
18.00	Alfa Aesar
17.50	Oxford University MSDS
17.50	PHYSPROP

octanenitrile C8H15N[3, 31, 64]

Compound Data



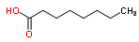
Melting point	**-45.53 °C**	**227.62 K**			
CSID	29026	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	125.2114	**H bond donors**	0	**ACD/LogP**	2.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	5	**Predicted density**	0.81 g/cm^3
SMILES	N#CCCCCCCC				
STD InChIKey	YSIMAPNUZAVQER-UHFFFAOYAQ				

Melting Points

mp °C	source
-45.00	Alfa Aesar
-46.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-45.60	PHYSPROP

octanoic acid C8H16O2[3, 4, 12, 32, 35, 64]

Compound Data

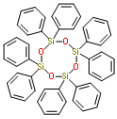


Melting point	**16.46 °C**	**289.61 K**			
CSID	370	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	144.2114	**H bond donors**	1	**ACD/LogP**	2.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.93 g/cm^3
SMILES	CCCCCCCC(=O)O				
STD InChIKey	WWZKQHOCKIZLMA-UHFFFAOYAH				

Melting Points

mp °C	source
17.00	Alfa Aesar
17.00	American Petroleum Institute. Research Project 44; Selected ...
15.85	Bond AD. New Journal of Chemistry 28 104-114 (2004)
16.30	DrugBank
16.30	EPISuite-ChemSpider
16.30	PHYSPROP

octaphenylcyclotetrasiloxane C48H40O4Si4



Compound Data

Melting point	**0.00 °C**	**273.15 K**			
CSID	61642	**H bond acceptors**	4	**Rule of 5 violations**	NA
Molecular weight	793.1708	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	1.22 g/cm^3
SMILES	O1[Si](O[Si](O[Si]1(c2ccccc2)c3ccccc3)(c4ccccc4)c5ccccc5)(c6ccccc6)c7ccccc7)(c8ccccc8)c9ccccc9				
STD InChIKey	VSIKJPJINIDELZ-UHFFFAOYAJ				

Melting Points

octyl cyanide C9H17N[31, 64]

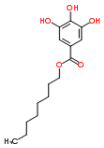
Compound Data

Melting point	**-34.10 °C**	**239.05 K**			
CSID	15846	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	139.238	**H bond donors**	0	**ACD/LogP**	3.27
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.82 g/cm^3
SMILES	N#CCCCCCCCC				
STD InChIKey	PLZZPPHAMDJOSR-UHFFFAOYAV				

Melting Points

mp °C	source
-34.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-34.20	PHYSPROP

octyl gallate C15H22O5[3, 64]



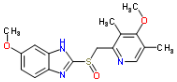
Compound Data

Melting point	**100.75 °C**	**373.90 K**			
CSID	55194	**H bond acceptors**	5	**Rule of 5 violations**	1
Molecular weight	282.3322	**H bond donors**	3	**ACD/LogP**	5.26
Phase 25 °C	solid	**Rotatable bonds**	12	**Predicted density**	1.19 g/cm^3
SMILES	O=C(OCCCCCCCC)c1cc(O)c(O)c(O)c1				
STD InChIKey	NRPKURNSADTHLJ-UHFFFAOYAL				

Melting Points

mp °C	source
99.00	Alfa Aesar
102.50	PHYSPROP

omeprazole C17H19N3O3S[9, 32, 32, 44, 48, 64]



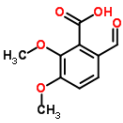
Compound Data

Melting point	**155.83 °C**	**428.98 K**			
CSID	4433	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	345.4161	**H bond donors**	1	**ACD/LogP**	2.17
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.37 g/cm^3
SMILES	O=S(c2nc1ccc(OC)cc1n2)Cc3ncc(c(OC)c3C)C				
STD InChIKey	SUBDBMMJDZJVOS-UHFFFAOYAZ				

Melting Points

mp °C	source
156.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
156.00	DrugBank
155.00	DrugBank
156.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
156.00	PHYSPROP

opianic acid C10H10O5[3, 64]



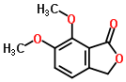
Compound Data

Melting point	**148.50 °C**	**421.65 K**			
CSID	61517	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	210.1834	**H bond donors**	1	**ACD/LogP**	0.63
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.30 g/cm^3
SMILES	O=Cc1ccc(OC)c(OC)c1C(=O)O				
STD InChIKey	HVXXOIGTXJOVON-UHFFFAOYAS				

Melting Points

mp °C	source
147.00	Alfa Aesar
150.00	PHYSPROP

opianyl C10H10O4[48, 64]



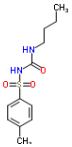
Compound Data

Melting point	**101.75 °C**	**374.90 K**			
CSID	61717	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.184	**H bond donors**	0	**ACD/LogP**	0.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.26 g/cm^3
SMILES	O=C1OCc2ccc(OC)c(OC)c12				
STD InChIKey	ORFFGRQMMWVHIB-UHFFFAOYAA				

Melting Points

mp °C	source
101.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
102.50	PHYSPROP

orinase C12H18N2O3S[3, 32, 61, 64]



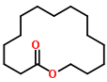
Compound Data

Melting point	**128.62 °C**	**401.77 K**			
CSID	5304	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	270.3479	**H bond donors**	2	**ACD/LogP**	2.34
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.18 g/cm^3
SMILES	O=S(=O)(c1ccc(cc1)C)NC(=O)NCCCC				
STD InChIKey	JLRGJRBPOGGCBT-UHFFFAOYAI				

Melting Points

mp °C	source
129.00	Alfa Aesar
128.50	DrugBank
128.50	Oxford University MSDS
128.50	PHYSPROP

oxacyclohexadecan-2-one C15H28O2[3, 64]



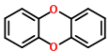
Compound Data

Melting point	**33.50 °C**	**306.65 K**			
CSID	205386	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	240.3816	**H bond donors**	0	**ACD/LogP**	5.44
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.89 g/cm^3
SMILES	O=C1OCCCCCCCCCCCCCC1				
STD InChIKey	FKUPPRZPSYCDRS-UHFFFAOYAJ				

Melting Points

mp °C	source
35.00	Alfa Aesar
32.00	PHYSPROP

oxanthrene C12H8O2[61, 64]



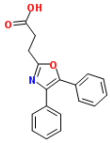
Compound Data

Melting point	**122.25 °C**	**395.40 K**			
CSID	8861	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	184.1907	**H bond donors**	0	**ACD/LogP**	4.38
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.24 g/cm^3
SMILES	O1c3c(Oc2c1cccc2)cccc3				
STD InChIKey	NFBOHOGPQUYFRF-UHFFFAOYAJ				

Melting Points

mp °C	source
122.50	Oxford University MSDS
122.00	PHYSPROP

oxaprozin C18H15NO3[9, 32, 64]



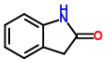
Compound Data

Melting point	**160.08 °C**	**433.23 K**			
CSID	4453	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	293.3166	**H bond donors**	1	**ACD/LogP**	3.89
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.22 g/cm^3
SMILES	O=C(O)CCc1nc(c(o1)c2ccccc2)c3ccccc3				
STD InChIKey	OFPXSFXSNFPTHF-UHFFFAOYAC				

Melting Points

mp °C	source
161.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
158.50	DrugBank
160.75	PHYSPROP

oxindole C8H7NO[3, 64]



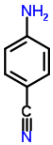
Compound Data

Melting point	**127.00 °C**	**400.15 K**			
CSID	284794	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	133.1473	**H bond donors**	1	**ACD/LogP**	1.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.20 g/cm^3
SMILES	c1ccc2c(c1)CC(=O)N2				
STD InChIKey	JYGFTBXVXVMTGB-UHFFFAOYAF				

Melting Points

mp °C	source
126.00	Alfa Aesar
128.00	PHYSPROP

p-cyanoaniline C7H6N2[2, 3, 64]



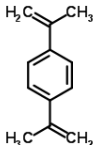
Compound Data

Melting point	**84.33 °C**	**357.48 K**			
CSID	12822	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1359	**H bond donors**	2	**ACD/LogP**	1.07
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.14 g/cm^3
SMILES	N#Cc1ccc(N)cc1				
STD InChIKey	YBAZINRZQSAIAY-UHFFFAOYAM				

Melting Points

mp °C	source
84.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
85.00	Alfa Aesar
84.00	PHYSPROP

p-diisopropenylbenzene C12H14[2, 64]



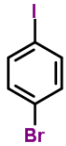
Compound Data

Melting point	**64.75 °C**	**337.90 K**			
CSID	66759	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	158.2396	**H bond donors**	0	**ACD/LogP**	4.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.87 g/cm^3
SMILES	C(/c1ccc(\C(=C)C)cc1)(=C)C				
STD InChIKey	ZENYUPUKNXGVDY-UHFFFAOYAU				

Melting Points

mp °C	source
66.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
63.50	PHYSPROP

p-iodobromobenzene C6H4BrI[2, 3, 64]



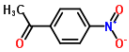
Compound Data

Melting point	**91.33 °C**	**364.48 K**			
CSID	11038	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	282.9044	**H bond donors**	0	**ACD/LogP**	3.95
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.21 g/cm^3
SMILES	Ic1ccc(Br)cc1				
STD InChIKey	UCCUXODGPMAHRL-UHFFFAOYAF				

Melting Points

mp °C	source
91.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
91.00	Alfa Aesar
92.00	PHYSPROP

p-nitroacetophenone C8H7NO3[2, 3, 64]



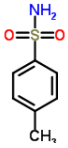
Compound Data

Melting point	**80.27 °C**	**353.42 K**			
CSID	21106581	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	165.1461	**H bond donors**	0	**ACD/LogP**	1.53
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	CC(=O)c1ccc(cc1)[N+](=O)[O-]				
STD InChIKey	YQYGPGKTNQNXMH-UHFFFAOYAV				

Melting Points

mp °C	source
80.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
79.00	Alfa Aesar
81.80	PHYSPROP

p-toluenesulfonamide C7H9NO2S[2, 3, 64]



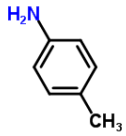
Compound Data

Melting point	**138.50 °C**	**411.65 K**			
CSID	6033	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	171.2169	**H bond donors**	2	**ACD/LogP**	0.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.27 g/cm^3
SMILES	O=S(=O)(c1ccc(cc1)C)N				
STD InChIKey	LMYRWZFENFIFIT-UHFFFAOYAF				

Melting Points

mp °C	source
139.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
138.00	Alfa Aesar
138.50	PHYSPROP

p-toluidine C7H9N[3, 31, 61, 64, 64]



Compound Data

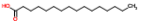
Melting point	**43.65 °C**	**316.80 K**			
CSID	13835151	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	107.1531	**H bond donors**	2	**ACD/LogP**	1.40
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.99 g/cm^3
SMILES	Cc1ccc(N)cc1				
STD InChIKey	RZXMPPFPUUCRFN-UHFFFAOYAP				

Melting Points

mp °C	source
44.00	Alfa Aesar
44.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
43.00	Oxford University MSDS
43.60	PHYSPROP
	Values not used in calculating the average melting point
244.00	PHYSPROP[1]

1. salt JCB

palmitic acid C16H32O2[3, 61, 64]



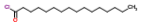
Compound Data

Melting point	**61.77 °C**	**334.92 K**			
CSID	960	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	256.4241	**H bond donors**	1	**ACD/LogP**	6.81
Phase 25 °C	solid	**Rotatable bonds**	14	**Predicted density**	0.89 g/cm^3
SMILES	CCCCCCCCCCCCCCCC(=O)O				
STD InChIKey	IPCSVZSSVZVIGE-UHFFFAOYAJ				

Melting Points

mp °C	source
61.00	Alfa Aesar
62.50	Oxford University MSDS
61.80	PHYSPROP

palmitoyl chloride C16H31ClO[3, 64]



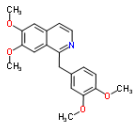
Compound Data

Melting point	**11.50 °C**	**284.65 K**			
CSID	7914	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	274.8697	**H bond donors**	0	**ACD/LogP**	7.90
Phase 25 °C	liquid/gas	**Rotatable bonds**	14	**Predicted density**	0.91 g/cm^3
SMILES	ClC(=O)CCCCCCCCCCCCCCC				
STD InChIKey	ARBOVOVUTSQWSS-UHFFFAOYAK				

Melting Points

mp °C	source
11.00	Alfa Aesar
12.00	PHYSPROP

papaverine C20H21NO4[3, 64]



Compound Data

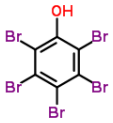
Melting point	**147.25 °C**	**420.40 K**			
CSID	4518	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	339.385	**H bond donors**	0	**ACD/LogP**	2.93
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.16 g/cm^3
SMILES	COc1ccc(cc1OC)Cc2c3cc(c(cc3ccn2)OC)OC				
STD InChIKey	XQYZDYMELSJDRZ-UHFFFAOYAJ				

Melting Points

mp °C	source
147.00	Alfa Aesar
147.50	PHYSPROP

pentabromophenol C6HBr5O[3, 61, 64]

Compound Data



Melting point	**228.50 °C**	**501.65 K**			
CSID	11359	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	488.5915	**H bond donors**	1	**ACD/LogP**	6.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.89 g/cm^3
SMILES	Brc1c(O)c(Br)c(Br)c(Br)c1Br				
STD InChIKey	SVHOVVJFOWGYJO-UHFFFAOYAU				

Melting Points

mp °C	source
226.00	Alfa Aesar
230.00	Oxford University MSDS
229.50	PHYSPROP

pentachloroaniline C6H2Cl5N[3, 64]

Compound Data

Melting point	**233.50 °C**	**506.65 K**			
CSID	10243	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	265.3518	**H bond donors**	2	**ACD/LogP**	4.86
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.75 g/cm^3
SMILES	Clc1c(c(Cl)c(Cl)c(Cl)c1Cl)N				
STD InChIKey	KHCZSJXTDDHLGJ-UHFFFAOYAH				

Melting Points

mp °C	source
232.00	Alfa Aesar
235.00	PHYSPROP

pentachlorophenol C6HCl5O[61, 64, 70, 72]

Compound Data

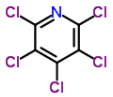
Melting point	**173.62 °C**	**446.77 K**			
CSID	967	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	266.3365	**H bond donors**	1	**ACD/LogP**	4.78
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.80 g/cm^3
SMILES	Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl				
STD InChIKey	IZUPBVBPLAPZRR-UHFFFAOYAG				

Melting Points

mp °C	source
174.00	Oxford University MSDS
174.00	PHYSPROP
174.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
172.50	Sigma-Aldrich

pentachloropyridine C5Cl5N[3, 64]

Compound Data



Melting point	**125.25 °C**	**398.40 K**			
CSID	15724	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	251.3252	**H bond donors**	0	**ACD/LogP**	3.60
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.76 g/cm^3
SMILES	Clc1c(Cl)c(Cl)nc(Cl)c1Cl				
STD InChIKey	DNDPLEAVNVOOQZ-UHFFFAOYAW				

Melting Points

mp °C	source
125.00	Alfa Aesar
125.50	PHYSPROP

pentacosane C25H52[3, 64]

Compound Data

Melting point	**53.50 °C**	**326.65 K**			
CSID	11900	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	352.6804	**H bond donors**	0	**ACD/LogP**	14.04
Phase 25 °C	solid	**Rotatable bonds**	22	**Predicted density**	0.80 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCC)CCCC				
STD InChIKey	YKNWIILGEFFOPE-UHFFFAOYAK				

Melting Points

mp °C	source
53.00	Alfa Aesar
54.00	PHYSPROP

pentadecafluorooctanoic acid C8HF15O2[61, 64]

Compound Data

Melting point	**54.90 °C**	**328.05 K**			
CSID	9180	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	414.0684	**H bond donors**	1	**ACD/LogP**	7.75
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.75 g/cm^3
SMILES	FC(F)(C(F)(F)C(=O)O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F				
STD InChIKey	SNGREZUHAYWORS-UHFFFAOYAQ				

Melting Points

mp °C	source
55.50	Oxford University MSDS
54.30	PHYSPROP

pentadecane C15H32[3, 4, 61, 64]

Compound Data

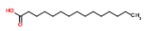
Melting point	**9.95 °C**	**283.10 K**			
CSID	11885	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	212.4146	**H bond donors**	0	**ACD/LogP**	8.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	12	**Predicted density**	0.77 g/cm^3
SMILES	C(CCCCCC)CCCCCCCC				
STD InChIKey	YCOZIPAWZNQLMR-UHFFFAOYAP				

Melting Points

mp °C	source
10.00	Alfa Aesar
10.00	American Petroleum Institute. Research Project 44; Selected ...
9.90	Oxford University MSDS
9.90	PHYSPROP

pentadecanoic acid C15H30O2[3, 61, 64]

Compound Data



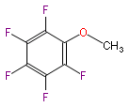
Melting point	**52.43 °C**	**325.58 K**			
CSID	13249	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	242.3975	**H bond donors**	1	**ACD/LogP**	6.62
Phase 25 °C	solid	**Rotatable bonds**	13	**Predicted density**	0.90 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCC				
STD InChIKey	WQEPLUUGTLDZJY-UHFFFAOYAK				

Melting Points

mp °C	source
53.00	Alfa Aesar
52.00	Oxford University MSDS
52.30	PHYSPROP

pentafluoroanisole C7H3F5O[3, 64]

Compound Data



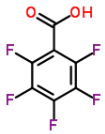
Melting point	**-37.50 °C**	**235.65 K**			
CSID	21171396	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	198.0901	**H bond donors**	0	**ACD/LogP**	2.39
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.47 g/cm^3
SMILES	Fc1c(F)c(F)c(F)c(F)c1OC				
STD InChIKey	ZRQUIRABLIQJRI-UHFFFAOYAM				

Melting Points

mp °C	source
-38.00	Alfa Aesar
-37.00	PHYSPROP

pentafluorobenzoic acid C7HF5O2[3, 64]

Compound Data



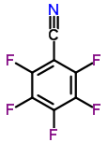
Melting point	**101.50 °C**	**374.65 K**			
CSID	11277	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	212.0737	**H bond donors**	1	**ACD/LogP**	2.46
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.72 g/cm^3
SMILES	Fc1c(c(F)c(F)c(F)c1F)C(=O)O				
STD InChIKey	YZERDTREOUSUHF-UHFFFAOYAQ				

Melting Points

mp °C	source
102.00	Alfa Aesar
101.00	PHYSPROP

pentafluorobenzonitrile C7F5N[3, 64]

Compound Data



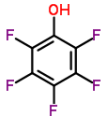
Melting point	**2.20 °C**	**275.35 K**			
CSID	63077	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	193.0736	**H bond donors**	0	**ACD/LogP**	0.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.55 g/cm^3
SMILES	Fc1c(C#N)c(F)c(F)c(F)c1F				
STD InChIKey	YXWJGZQOGXGSSC-UHFFFAOYAJ				

Melting Points

mp °C	source
2.00	Alfa Aesar
2.40	PHYSPROP

pentafluorophenol C6HF5O[3, 61, 64]

Compound Data



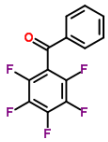
Melting point	**33.93 °C**	**307.08 K**			
CSID	12499	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	184.0636	**H bond donors**	1	**ACD/LogP**	3.05
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.69 g/cm^3
SMILES	Fc1c(F)c(F)c(F)c(O)c1F				
STD InChIKey	XBNGYFFABRKICK-UHFFFAOYAG				

Melting Points

mp °C	source
34.00	Alfa Aesar
35.00	Oxford University MSDS
32.80	PHYSPROP

pentafluorophenyl phenyl ketone C13H5F5O[3, 61, 64]

Compound Data



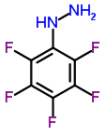
Melting point	**37.50 °C**	**310.65 K**			
CSID	66396	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	272.1702	**H bond donors**	0	**ACD/LogP**	2.29
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.44 g/cm^3
SMILES	Fc1c(c(F)c(F)c(F)c1F)C(=O)c2ccccc2				
STD InChIKey	HCCPWBWOSASKLG-UHFFFAOYAF				

Melting Points

mp °C	source
38.00	Alfa Aesar
37.50	Oxford University MSDS
37.00	PHYSPROP

pentafluorophenylhydrazine C6H3F5N2[3, 64]

Compound Data



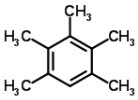
Melting point	**75.50 °C**	**348.65 K**			
CSID	12681	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.0934	**H bond donors**	3	**ACD/LogP**	2.52
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.69 g/cm^3
SMILES	Fc1c(F)c(F)c(F)c(F)c1NN				
STD InChIKey	BYCUWCJUPSUFBX-UHFFFAOYAP				

Melting Points

mp °C	source
76.00	Alfa Aesar
75.00	PHYSPROP

pentamethylbenzene C11H16[4, 64]

Compound Data



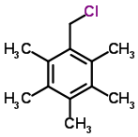
Melting point	**54.25 °C**	**327.40 K**			
CSID	12259	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	148.2447	**H bond donors**	0	**ACD/LogP**	4.52
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	c1(c(cc(c(c1C)C)C)C)C				
STD InChIKey	BEZDDPMMPIDMGJ-UHFFFAOYAT				

Melting Points

mp °C	source
54.00	American Petroleum Institute. Research Project 44; Selected ...
54.50	PHYSPROP

pentamethylbenzyl chloride C12H17Cl[3, 48]

Compound Data



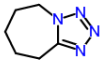
Melting point	**82.50 °C**	**355.65 K**			
CSID	61399	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	196.7164	**H bond donors**	0	**ACD/LogP**	4.79
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.99 g/cm^3
SMILES	ClCc1c(c(c(c(c1C)C)C)C)C				
STD InChIKey	CXUAEBDTJFKMBV-UHFFFAOYAP				

Melting Points

mp °C	source
83.00	Alfa Aesar
82.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

pentamethylenetetrazol C6H10N4[3, 61, 64]

Compound Data



Melting point	**59.00 °C**	**332.15 K**			
CSID	5704	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	138.1704	**H bond donors**	0	**ACD/LogP**	0.14
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	n1nnc2n1CCCCC2				
STD InChIKey	CWRVKFFCRWGWCS-UHFFFAOYAS				

Melting Points

mp °C	source
60.00	Alfa Aesar
57.50	Oxford University MSDS
59.50	PHYSPROP

pentane C5H12[3, 4, 15, 61, 64]

Compound Data

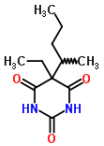
Melting point	**-129.89 °C**	**143.26 K**			
CSID	7712	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	72.1488	**H bond donors**	0	**ACD/LogP**	3.41
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.65 g/cm^3
SMILES	CCCCC				
STD InChIKey	OFBQJSOFQDEBGM-UHFFFAOYAN				

Melting Points

mp °C	source
-130.00	Alfa Aesar
-130.00	American Petroleum Institute. Research Project 44; Selected ...
-129.73	Carruth GF; Kobayahsi R. Journal of Chemical and Engineering...
-130.00	Oxford University MSDS
-129.70	PHYSPROP

pentobarbital C11H18N2O3[32, 35, 44, 64]

Compound Data



Melting point	**129.62 °C**	**402.77 K**			
CSID	4575	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	226.2722	**H bond donors**	2	**ACD/LogP**	2.05
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.08 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(C(C)CCC)CC				
STD InChIKey	WEXRUCMBJFQVBZ-UHFFFAOYAD				

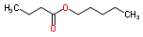
Melting Points

mp °C	source
129.50	DrugBank
129.50	EPISuite-ChemSpider
129.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
130.00	PHYSPROP

pentyl butyrate C9H18O2[7, 64]

Compound Data

Melting point	**-73.10 °C**	**200.05 K**			
CSID	10428	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.238	**H bond donors**	0	**ACD/LogP**	3.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	3



0.88 g/cm

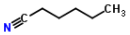
SMILES	O=C(OCCCCC)CCC
STD InChIKey	CFNJLPHOBMVMNS-UHFFFAOYAQ

Melting Points

mp °C	source
-73.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
-73.20	PHYSPROP

pentyl cyanide C6H11N[31, 64]

Compound Data



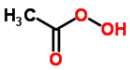
Melting point	**-80.15 °C**	**193.00 K**			
CSID	11846	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	97.1582	**H bond donors**	0	**ACD/LogP**	1.68
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.80 g/cm^3
SMILES	N#CCCCCC				
STD InChIKey	AILKHAQXUAOOFU-UHFFFAOYAZ				

Melting Points

mp °C	source
-80.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-80.30	PHYSPROP

peracetic acid C2H4O3[61, 64]

Compound Data



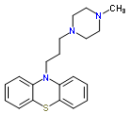
Melting point	**-0.05 °C**	**273.10 K**			
CSID	6336	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	76.0514	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.22 g/cm^3
SMILES	CC(=O)OO				
STD InChIKey	KFSLWBXXFJQRDL-UHFFFAOYAD				

Melting Points

mp °C	source
0.10	Oxford University MSDS
-0.20	PHYSPROP

perazine C20H25N3S[44, 64]

Compound Data



Melting point	**52.50 °C**	**325.65 K**			
CSID	4582	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	339.4976	**H bond donors**	0	**ACD/LogP**	4.04
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.15 g/cm^3
SMILES	S2c1ccccc1N(c3c2cccc3)CCCN4CCN(C)CC4				
STD InChIKey	WEYVCQFUGFRXOM-UHFFFAOYAC				

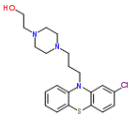
Melting Points

mp °C	source
53.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
52.00	PHYSPROP

perphenazine C21H26ClN3OS[9, 44, 48, 64]

Compound Data

Melting point	**95.47 °C**	**368.62 K**			
CSID	4586	**H bond acceptors**	4	**Rule of 5 violations**	0



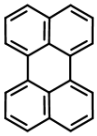
Molecular weight	403.9686	**H bond donors**	1	**ACD/LogP**	4.34
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.25 g/cm^3
SMILES	Clc2cc1N(c3c(Sc1cc2)cccc3)CCCN4CCN(CCO)CC4				
STD InChIKey	RGCVKNLCSQQDEP-UHFFFAOYAP				

Melting Points

mp °C	source
94.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
96.90	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
94.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
97.00	PHYSPROP

perylene C20H12[3, 44, 61, 64, 70]

Compound Data



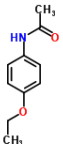
Melting point	**276.10 °C**	**549.25 K**			
CSID	8788	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	252.3093	**H bond donors**	0	**ACD/LogP**	6.19
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.29 g/cm^3
SMILES	c1cc2cccc3c2c(c1)c4cccc5c4c3ccc5				
STD InChIKey	CSHWQDPOILHKBI-UHFFFAOYAD				

Melting Points

mp °C	source
278.00	Alfa Aesar
273.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
278.00	Oxford University MSDS
274.00	PHYSPROP
277.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

phenacetin C10H13NO2[2, 3, 32, 35, 44, 61, 64, 70]

Compound Data



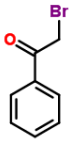
Melting point	**135.43 °C**	**408.57 K**			
CSID	4590	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	179.2157	**H bond donors**	1	**ACD/LogP**	1.63
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.10 g/cm^3
SMILES	O=C(Nc1ccc(OCC)cc1)C				
STD InChIKey	CPJSUEIXXCENMM-UHFFFAOYAO				

Melting Points

mp °C	source
135.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
135.00	Alfa Aesar
135.00	DrugBank
137.50	EPISuite-ChemSpider
134.40	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
134.00	Oxford University MSDS
137.50	PHYSPROP
135.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

phenacyl bromide C8H7BrO[3, 48, 64]

Compound Data



Melting point	**49.83 °C**	**322.98 K**			
CSID	6023	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	199.0446	**H bond donors**	0	**ACD/LogP**	2.19
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.48 g/cm^3
SMILES	O=C(c1ccccc1)CBr				

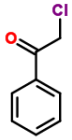
STD InChIKey	LIGACIXOYTUXAW-UHFFFAOYAV

Melting Points

mp °C	source
50.00	Alfa Aesar
49.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
50.50	PHYSPROP

phenacyl chloride C8H7ClO[3, 32, 61, 64]

Compound Data



Melting point	**55.17 °C**	**328.32 K**			
CSID	10303	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	154.5936	**H bond donors**	0	**ACD/LogP**	1.85
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=C(c1ccccc1)CCl				
STD InChIKey	IMACFCSSMIZSPP-UHFFFAOYAN				

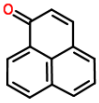
Melting Points

mp °C	source
54.00	Alfa Aesar
55.00	Oxford University MSDS
56.50	PHYSPROP
	Values not used in calculating the average melting point
-93.40	DrugBank[1]

1. incorrect SMILES - mp for methylamine JCB

phenalenone C13H8O[61, 64]

Compound Data



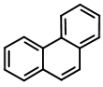
Melting point	**154.25 °C**	**427.40 K**			
CSID	10582	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	180.202	**H bond donors**	0	**ACD/LogP**	3.45
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	O=C3/C=C\c2cccc1cccc3c12				
STD InChIKey	WWBGWPHHLRSTFI-UHFFFAOYAL				

Melting Points

mp °C	source
154.50	Oxford University MSDS
154.00	PHYSPROP

phenanthrene C14H10[3, 35, 44, 61, 64, 70, 70]

Compound Data

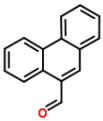


Melting point	**99.35 °C**	**372.50 K**			
CSID	970	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	178.2292	**H bond donors**	0	**ACD/LogP**	4.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.13 g/cm^3
SMILES	c1ccc2c(c1)ccc3c2cccc3				
STD InChIKey	YNPNZTXNASCQKK-UHFFFAOYAC				

Melting Points

mp °C	source
99.00	Alfa Aesar
99.20	EPISuite-ChemSpider
100.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
100.00	Oxford University MSDS
99.24	PHYSPROP
99.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
99.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

phenanthrene-9-carboxaldehyde C15H10O[3, 72]



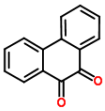
Compound Data

Melting point	**101.75 °C**	**374.90 K**			
CSID	70806	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	206.2393	**H bond donors**	0	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	O=Cc2cc3c(c1c2cccc1)cccc3				
STD InChIKey	QECIGCMPORCORE-UHFFFAOYAE				

Melting Points

mp °C	source
102.00	Alfa Aesar
101.50	Sigma-Aldrich

phenanthrene-9,10-dione C14H8O2[3, 48, 61, 64]



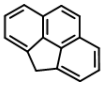
Compound Data

Melting point	**208.75 °C**	**481.90 K**			
CSID	6505	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	208.2121	**H bond donors**	0	**ACD/LogP**	2.69
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.31 g/cm^3
SMILES	c1ccc2c(c1)-c3ccccc3C(=O)C2=O				
STD InChIKey	YYVYAPXYZVYDHN-UHFFFAOYAF				

Melting Points

mp °C	source
210.00	Alfa Aesar
206.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
210.00	Oxford University MSDS
209.00	PHYSPROP

phenanthrindene C15H10[61, 64]



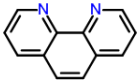
Compound Data

Melting point	**115.00 °C**	**388.15 K**			
CSID	8793	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	190.2399	**H bond donors**	0	**ACD/LogP**	4.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	c23ccc1cccc4c1c2c(ccc3)C4				
STD InChIKey	RKZDZWJDQTZDLD-UHFFFAOYAY				

Melting Points

mp °C	source
116.00	Oxford University MSDS
114.00	PHYSPROP

phenanthroline C12H8N2[3, 32, 64]



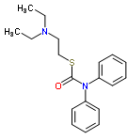
Compound Data

Melting point	**117.33 °C**	**390.48 K**			
CSID	1278	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	180.2053	**H bond donors**	0	**ACD/LogP**	2.25
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.25 g/cm^3
SMILES	c1cc2ccc3cccnc3c2nc1				
STD InChIKey	DGEZNRSVGBDHLK-UHFFFAOYAW				

Melting Points

mp °C	source
118.00	Alfa Aesar
117.00	DrugBank
117.00	PHYSPROP

phencarbamide C19H24N2OS[9, 48, 64]



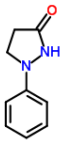
Compound Data

Melting point	**48.17 °C**	**321.32 K**			
CSID	5786	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	328.4717	**H bond donors**	0	**ACD/LogP**	4.99
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.13 g/cm^3
SMILES	O=C(SCCN(CC)CC)N(c1ccccc1)c2ccccc2				
STD InChIKey	BZGIPVGCJGXQTA-UHFFFAOYAO				

Melting Points

mp °C	source
48.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
48.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
48.50	PHYSPROP

phenidone C9H10N2O[3, 61, 64]



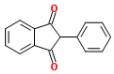
Compound Data

Melting point	**123.33 °C**	**396.48 K**			
CSID	6823	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	162.1885	**H bond donors**	1	**ACD/LogP**	0.18
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.19 g/cm^3
SMILES	O=C2NN(c1ccccc1)CC2				
STD InChIKey	CMCWWLVWPDLCRM-UHFFFAOYAF				

Melting Points

mp °C	source
122.00	Alfa Aesar
122.00	Oxford University MSDS
126.00	PHYSPROP

phenindione C15H10O2[32, 64]



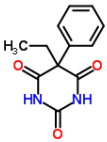
Compound Data

Melting point	**149.75 °C**	**422.90 K**			
CSID	4596	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	222.2387	**H bond donors**	0	**ACD/LogP**	3.30
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	O=C2c1ccccc1C(=O)C2c3ccccc3				
STD InChIKey	NFBAXHOPROOJAW-UHFFFAOYAZ				

Melting Points

mp °C	source
149.50	DrugBank
150.00	PHYSPROP

phenobarbital C12H12N2O3[32, 35, 44, 64, 70]



Compound Data

Melting point	**174.60 °C**	**447.75 K**			
CSID	4599	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	232.2353	**H bond donors**	2	**ACD/LogP**	1.67
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.23 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(c2ccccc2)CC				
STD InChIKey	DDBREPKUVSBGFI-UHFFFAOYAB				

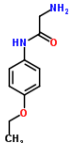
Melting Points

mp °C	source
174.00	DrugBank
174.00	EPISuite-ChemSpider
175.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...

174.00	PHYSPROP
176.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

phenocoll C10H14N2O2[9, 48, 64]

Compound Data



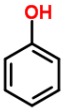
Melting point	**100.83 °C 373.98 K**				
CSID	60263	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	194.2304	**H bond donors**	3	**ACD/LogP**	0.03
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.17 g/cm^3
SMILES	O=C(Nc1ccc(OCC)cc1)CN				
STD InChIKey	LQJARUQXWJSDFL-UHFFFAOYAV				

Melting Points

mp °C	source
101.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
101.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
100.50	PHYSPROP

phenol C6H6O[3, 31, 64, 70, 72]

Compound Data



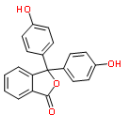
Melting point	**41.18 °C 314.33 K**				
CSID	971	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	94.1112	**H bond donors**	1	**ACD/LogP**	1.54
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.07 g/cm^3
SMILES	c1ccc(cc1)O				
STD InChIKey	ISWSIDIOOBJBQZ-UHFFFAOYAI				

Melting Points

mp °C	source
42.00	Alfa Aesar
41.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
40.90	PHYSPROP
41.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
41.00	Sigma-Aldrich

phenolphthalein C20H14O4[3, 32, 44, 64]

Compound Data



Melting point	**261.25 °C 534.40 K**				
CSID	4600	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	318.3228	**H bond donors**	2	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.39 g/cm^3
SMILES	O=C1OC(c2ccccc12)(c3ccc(O)cc3)c4ccc(O)cc4				
STD InChIKey	KJFMBFZCATUALV-UHFFFAOYAH				

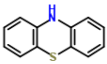
Melting Points

mp °C	source
260.00	Alfa Aesar
262.50	DrugBank
260.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
262.50	PHYSPROP

phenothiazine C12H9NS[3, 3, 28, 56, 64, 72, 72]

Compound Data

Melting point	**185.30 °C 458.45 K**				
CSID	21106365	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	199.2716	**H bond donors**	1	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3



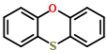
SMILES	c1ccc2c(c1)Nc3ccccc3S2
STD InChIKey	WJFKNYWRSNBZNX-UHFFFAOYAI

Melting Points

mp °C	source
183.50	Alfa Aesar
184.00	Alfa Aesar
187.50	CRC Handbook of Chemistry and Physics
185.10	Merck Index
187.50	PHYSPROP
184.50	Sigma-Aldrich
185.00	Sigma-Aldrich

phenoxathiine C12H8OS[3, 61]

Compound Data



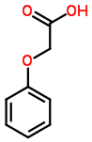
Melting point	**58.25 °C**	**331.40 K**			
CSID	8862	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	200.2563	**H bond donors**	0	**ACD/LogP**	4.54
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.28 g/cm^3
SMILES	O1c3c(Sc2c1cccc2)cccc3				
STD InChIKey	GJSGGHOYGKMUPT-UHFFFAOYAV				

Melting Points

mp °C	source
57.00	Alfa Aesar
59.50	Oxford University MSDS

phenoxyacetic acid C8H8O3[2, 3, 64]

Compound Data



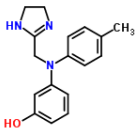
Melting point	**99.50 °C**	**372.65 K**			
CSID	18107	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.34
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	O=C(O)COc1ccccc1				
STD InChIKey	LCPDWSOZIOUXRV-UHFFFAOYAQ				

Melting Points

mp °C	source
100.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
100.00	Alfa Aesar
98.50	PHYSPROP

phentolamine C17H19N3O[32, 64]

Compound Data



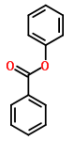
Melting point	**174.75 °C**	**447.90 K**			
CSID	5571	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	281.3523	**H bond donors**	2	**ACD/LogP**	3.60
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.18 g/cm^3
SMILES	Oc3cc(N(c1ccc(cc1)C)CC/2=N/CCN\2)ccc3				
STD InChIKey	MRBDMNSDAVCSSF-UHFFFAOYAI				

Melting Points

mp °C	source
174.50	DrugBank
175.00	PHYSPROP

phenyl benzoate C13H10O2[2, 3, 48, 64, 72]

Compound Data



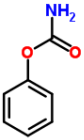
Melting point	**69.20 °C**	**342.35 K**			
CSID	6901	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2173	**H bond donors**	0	**ACD/LogP**	3.59
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.15 g/cm^3
SMILES	O=C(Oc1ccccc1)c2ccccc2				
STD InChIKey	FCJSHPDYVMKCHI-UHFFFAOYAU				

Melting Points

mp °C	source
70.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
69.00	Alfa Aesar
67.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
71.00	PHYSPROP
69.00	Sigma-Aldrich

phenyl carbamate C7H7NO2[3, 64]

Compound Data



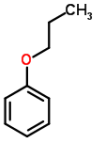
Melting point	**150.50 °C**	**423.65 K**			
CSID	62532	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	137.136	**H bond donors**	2	**ACD/LogP**	1.08
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.20 g/cm^3
SMILES	O=C(Oc1ccccc1)N				
STD InChIKey	BSCCSDNZEIHXOK-UHFFFAOYAJ				

Melting Points

mp °C	source
151.00	Alfa Aesar
150.00	PHYSPROP

phenyl propyl ether C9H12O[7, 64]

Compound Data



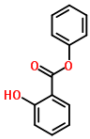
Melting point	**-27.50 °C**	**245.65 K**			
CSID	11655	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	136.191	**H bond donors**	0	**ACD/LogP**	3.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.93 g/cm^3
SMILES	O(c1ccccc1)CCC				
STD InChIKey	DSNYFFJTZPIKFZ-UHFFFAOYAJ				

Melting Points

mp °C	source
-28.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
-27.00	PHYSPROP

phenyl salicylate C13H10O3[3, 35, 64, 67, 72]

Compound Data



Melting point	**42.40 °C**	**315.55 K**			
CSID	8058	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.2167	**H bond donors**	1	**ACD/LogP**	3.55
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=C(Oc1ccccc1)c2ccccc2O				
STD InChIKey	ZQBAKBUEJOMQEX-UHFFFAOYAI				

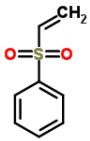
Melting Points

mp °C	source
43.00	Alfa Aesar
42.20	RTC melting point standard

42.00	Sigma-Aldrich
	Values not used in calculating the average melting point
130.50	EPISuite-ChemSpider[1]
130.50	PHYSPROP[2]

1. clearly out of range JCB
2. clearly out of range JCB

phenyl vinyl sulfone C8H8O2S[3, 61]



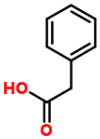
Compound Data

Melting point	**68.50 °C**	**341.65 K**			
CSID	71964	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	168.2129	**H bond donors**	0	**ACD/LogP**	1.20
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.18 g/cm^3
SMILES	O=S(=O)(\C=C)c1ccccc1				
STD InChIKey	UJTPZISIAWDGFF-UHFFFAOYAS				

Melting Points

mp °C	source
69.00	Alfa Aesar
68.00	Oxford University MSDS

phenylacetic acid C8H8O2[2, 3, 3, 35, 48, 59, 64, 72]



Compound Data

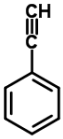
Melting point	**77.17 °C**	**350.32 K**			
CSID	10181341	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	136.1479	**H bond donors**	1	**ACD/LogP**	1.50
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	O=C(O)Cc1ccccc1				
STD InChIKey	WLJVXDMOQOGPHL-UHFFFAOYAR				

Melting Points

mp °C	source
79.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
77.50	Alfa Aesar
77.50	Alfa Aesar
76.70	EPISuite-ChemSpider
76.00	NIST Web Book
76.50	PHYSPROP
77.00	Sigma-Aldrich
	Values not used in calculating the average melting point
150.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...[1]

1. clearly out of range JCB

phenylacetylene C8H6[3, 64]



Compound Data

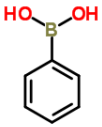
Melting point	**-44.90 °C**	**228.25 K**			
CSID	10364	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	102.1332	**H bond donors**	0	**ACD/LogP**	2.70
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.95 g/cm^3
SMILES	C#Cc1ccccc1				
STD InChIKey	UEXCJVNBTNXOEH-UHFFFAOYAC				

Melting Points

mp °C	source
-45.00	Alfa Aesar
-44.80	PHYSPROP

3, 64

phenylboronic acid C6H7BO2



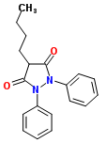
Compound Data

Melting point	**218.00 °C**	**491.15 K**			
CSID	60191	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	121.9296	**H bond donors**	2	**ACD/LogP**	1.24
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.14 g/cm^3
SMILES	B(c1ccccc1)(O)O				
STD InChIKey	HXITXNWTGFUOAU-UHFFFAOYAQ				

Melting Points

mp °C	source
217.00	Alfa Aesar
219.00	PHYSPROP

phenylbutazone C19H20N2O2[3, 32, 44, 64]



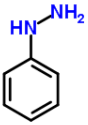
Compound Data

Melting point	**105.50 °C**	**378.65 K**			
CSID	4617	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	308.3743	**H bond donors**	0	**ACD/LogP**	3.16
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.17 g/cm^3
SMILES	O=C2N(c1ccccc1)N(C(=O)C2CCCC)c3ccccc3				
STD InChIKey	VYMDGNCVAMGZFE-UHFFFAOYAL				

Melting Points

mp °C	source
107.00	Alfa Aesar
105.00	DrugBank
105.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
105.00	PHYSPROP

phenylhydrazine C6H8N2[3, 64]



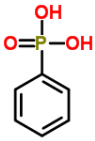
Compound Data

Melting point	**19.30 °C**	**292.45 K**			
CSID	7235	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	108.1411	**H bond donors**	3	**ACD/LogP**	1.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.12 g/cm^3
SMILES	NNc1ccccc1				
STD InChIKey	HKOOXMFOFWEVGF-UHFFFAOYAN				

Melting Points

mp °C	source
19.00	Alfa Aesar
19.60	PHYSPROP

phenylphosphonic acid C6H7O3P[3, 64]



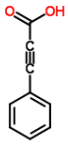
Compound Data

Melting point	**162.75 °C**	**435.90 K**			
CSID	14560	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	158.0917	**H bond donors**	2	**ACD/LogP**	0.54
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.42 g/cm^3
SMILES	O=P(O)(O)c1ccccc1				
STD InChIKey	QLZHNIAADXEJJP-UHFFFAOYAC				

Melting Points

mp °C	source
161.00	Alfa Aesar
164.50	PHYSPROP

phenylpropiolic acid C9H6O2[3, 3]



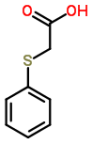
Compound Data

Melting point	**136.50 °C**	**409.65 K**			
CSID	62682	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	146.1427	**H bond donors**	1	**ACD/LogP**	2.61
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.24 g/cm^3
SMILES	O=C(C#Cc1ccccc1)O				
STD InChIKey	XNERWVPQCYSMLC-UHFFFAOYAX				

Melting Points

mp °C	source
136.00	Alfa Aesar
137.00	Alfa Aesar

phenylthioacetic acid C8H8O2S[3, 64]



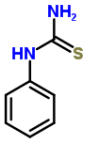
Compound Data

Melting point	**64.50 °C**	**337.65 K**			
CSID	53706	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	168.2129	**H bond donors**	1	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.27 g/cm^3
SMILES	O=C(O)CSc1ccccc1				
STD InChIKey	MOTOSAGBNXXRRE-UHFFFAOYAI				

Melting Points

mp °C	source
64.00	Alfa Aesar
65.00	PHYSPROP

phenylthiourea C7H8N2S[61, 64]



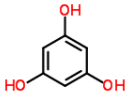
Compound Data

Melting point	**151.50 °C**	**424.65 K**			
CSID	589165	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	152.2168	**H bond donors**	3	**ACD/LogP**	0.73
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	S=C(Nc1ccccc1)N				
STD InChIKey	FULZLIGZKMKICU-UHFFFAOYAW				

Melting Points

mp °C	source
149.00	Oxford University MSDS
154.00	PHYSPROP

phloroglucinol C6H6O3[3, 64]



Compound Data

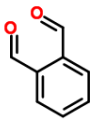
Melting point	**218.25 °C**	**491.40 K**			
CSID	352	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	126.11	**H bond donors**	3	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.49 g/cm^3
SMILES	c1c(cc(cc1O)O)O				
STD InChIKey	QCDYQQDYXPDABM-UHFFFAOYAF				

Melting Points

mp °C	source
218.00	Alfa Aesar
218.50	PHYSPROP

phthalaldehyde C8H6O2[2, 61, 64]

Compound Data



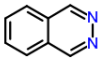
Melting point	**56.17 °C**	**329.32 K**			
CSID	4642	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	134.132	**H bond donors**	0	**ACD/LogP**	0.51
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	O=Cc1ccccc1C=O				
STD InChIKey	ZWLUXSQADUDCSB-UHFFFAOYAD				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
56.00	Oxford University MSDS
56.50	PHYSPROP

phthalazine C8H6N2[3, 64]

Compound Data



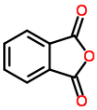
Melting point	**90.75 °C**	**363.90 K**			
CSID	8852	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1466	**H bond donors**	0	**ACD/LogP**	0.46
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.18 g/cm^3
SMILES	n2ncc1ccccc1c2				
STD InChIKey	LFSXCDWNBUNEEM-UHFFFAOYAE				

Melting Points

mp °C	source
91.00	Alfa Aesar
90.50	PHYSPROP

phthalic anhydride C8H4O3[3, 64]

Compound Data



Melting point	**131.40 °C**	**404.55 K**			
CSID	6552	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	148.1156	**H bond donors**	0	**ACD/LogP**	1.60
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.44 g/cm^3
SMILES	O=C1OC(=O)c2ccccc12				
STD InChIKey	LGRFSURHDFAFJT-UHFFFAOYAZ				

Melting Points

mp °C	source
132.00	Alfa Aesar
130.80	PHYSPROP

phthalide C8H6O2[3, 64]

Compound Data

Melting point	**74.50 °C**	**347.65 K**			
CSID	6621	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	134.132	**H bond donors**	0	**ACD/LogP**	0.99
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	O=C1OCc2ccccc12				
STD InChIKey	WNZQDUSMALZDQF-UHFFFAOYAW				

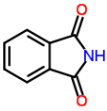
Melting Points

mp °C	source
74.00	Alfa Aesar
75.00	PHYSPROP

phthalimide C8H5NO2[3, 64]

Compound Data

Melting point	**236.00 °C**	**509.15 K**



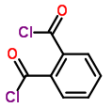
CSID	6550	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	147.1308	**H bond donors**	1	**ACD/LogP**	1.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.37 g/cm^3
SMILES	O=C2c1ccccc1C(=O)N2				
STD InChIKey	XKJCHHZQLQNZHY-UHFFFAOYAS				

Melting Points

mp °C	source
234.00	Alfa Aesar
238.00	PHYSPROP

phthaloyl chloride C8H4Cl2O2[3, 64]

Compound Data



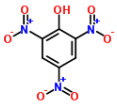
Melting point	**13.75 °C**	**286.90 K**			
CSID	13865683	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	203.0222	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.43 g/cm^3
SMILES	O=C(Cl)c1ccccc1C(Cl)=O				
STD InChIKey	FYXKZNLBZKRYSS-UHFFFAOYAB				

Melting Points

mp °C	source
12.00	Alfa Aesar
15.50	PHYSPROP

picric acid C6H3N3O7[61, 64]

Compound Data



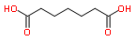
Melting point	**122.25 °C**	**395.40 K**			
CSID	6688	**H bond acceptors**	10	**Rule of 5 violations**	1
Molecular weight	229.1039	**H bond donors**	1	**ACD/LogP**	1.84
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.86 g/cm^3
SMILES	O=[N+]([O-])c1cc(cc([N+]([O-])=O)c1O)[N+]([O-])=O				
STD InChIKey	OXNIZHLAWKMVMX-UHFFFAOYAM				

Melting Points

mp °C	source
122.00	Oxford University MSDS
122.50	PHYSPROP

pimelic acid C7H12O4[3, 32, 64]

Compound Data



Melting point	**105.33 °C**	**378.48 K**			
CSID	376	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	160.1678	**H bond donors**	2	**ACD/LogP**	0.27
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.20 g/cm^3
SMILES	O=C(O)CCCCCC(=O)O				
STD InChIKey	WLJVNTCWHIRURA-UHFFFAOYAR				

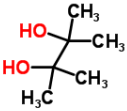
Melting Points

mp °C	source
104.00	Alfa Aesar
106.00	DrugBank
106.00	PHYSPROP

pinacol C6H14O2[2, 3, 64]

Compound Data

Melting point	**43.33 °C**	**316.48 K**	



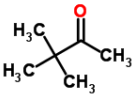
CSID	21109330	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	118.1742	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.96 g/cm^3
SMILES	CC(C)(O)C(C)(C)O				
STD InChIKey	IVDFJHOHABJVEH-UHFFFAOYAX				

Melting Points

mp °C	source
43.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
44.00	Alfa Aesar
43.00	PHYSPROP

pinacolone C6H12O[3, 4, 61, 64]

Compound Data



Melting point	**-52.50 °C**	**220.65 K**			
CSID	6176	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	100.1589	**H bond donors**	0	**ACD/LogP**	1.07
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.80 g/cm^3
SMILES	O=C(C)C(C)(C)C				
STD InChIKey	PJGSXYOJTGTZAV-UHFFFAOYAH				

Melting Points

mp °C	source
-53.00	Alfa Aesar
-52.00	American Petroleum Institute. Research Project 44; Selected ...
-52.50	Oxford University MSDS
-52.50	PHYSPROP

piperazine C4H10N2[3, 32, 64]

Compound Data

Melting point	**107.33 °C**	**380.48 K**			
CSID	13835459	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	86.1356	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	C1CNCCN1				
STD InChIKey	GLUUGHFHXGJENI-UHFFFAOYAS				

Melting Points

mp °C	source
110.00	Alfa Aesar
106.00	DrugBank
106.00	PHYSPROP

piperidine C5H11N[3, 64]

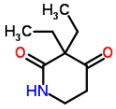
Compound Data

Melting point	**-9.00 °C**	**264.15 K**			
CSID	7791	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	85.1475	**H bond donors**	1	**ACD/LogP**	0.61
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.83 g/cm^3
SMILES	C1CCNCC1				
STD InChIKey	NQRYJNQNLNOLGT-UHFFFAOYAY				

Melting Points

mp °C	source
-11.00	Alfa Aesar
-7.00	PHYSPROP

piperidione C9H15NO2[9, 48, 64]



Compound Data

Melting point	**102.67 °C**	**375.82 K**			
CSID	6222	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	169.2209	**H bond donors**	1	**ACD/LogP**	-0.27
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.00 g/cm^3
SMILES	O=C1C(C(=O)NCC1)(CC)CC				
STD InChIKey	RGEVWUKXWFOAID-UHFFFAOYAK				

Melting Points

mp °C	source
102.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
102.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
104.00	PHYSPROP

piperidone C5H9NO[3, 64]

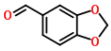
Compound Data

Melting point	**38.25 °C**	**311.40 K**			
CSID	12144	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	99.1311	**H bond donors**	1	**ACD/LogP**	-0.89
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	O=C1NCCCC1				
STD InChIKey	XUWHAWMETYGRKB-UHFFFAOYAE				

Melting Points

mp °C	source
37.00	Alfa Aesar
39.50	PHYSPROP

piperonal C8H6O3[3, 35, 64]



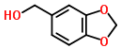
Compound Data

Melting point	**36.67 °C**	**309.82 K**			
CSID	13859497	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	150.1314	**H bond donors**	0	**ACD/LogP**	1.05
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	c1cc2c(cc1C=O)OCO2				
STD InChIKey	SATCULPHIDQDRE-UHFFFAOYAS				

Melting Points

mp °C	source
36.00	Alfa Aesar
37.00	EPISuite-ChemSpider
37.00	PHYSPROP

piperonol C8H8O3[3, 64]



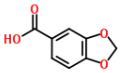
Compound Data

Melting point	**55.50 °C**	**328.65 K**			
CSID	9900	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	0.90
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O1c2ccc(cc2OC1)CO				
STD InChIKey	BHUIUXNAPJIDOG-UHFFFAOYAA				

Melting Points

mp °C	source
53.00	Alfa Aesar
58.00	PHYSPROP

piperonylic acid C8H6O4[3, 64]



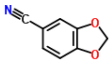
Compound Data

Melting point	**231.00 °C**	**504.15 K**			
CSID	6928	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	166.1308	**H bond donors**	1	**ACD/LogP**	2.01
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.47 g/cm^3
SMILES	O=C(O)c1ccc2OCOc2c1				
STD InChIKey	VDVJGIYXDVPQLP-UHFFFAOYAN				

Melting Points

mp °C	source
233.00	Alfa Aesar
229.00	PHYSPROP

piperonylonitrile C8H5NO2[3, 48]



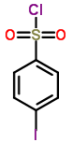
Compound Data

Melting point	**93.50 °C**	**366.65 K**			
CSID	70512	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	147.1308	**H bond donors**	0	**ACD/LogP**	1.88
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.34 g/cm^3
SMILES	N#Cc1ccc2OCOc2c1				
STD InChIKey	PKRWWZCDLJSJIF-UHFFFAOYAP				

Melting Points

mp °C	source
93.00	Alfa Aesar
94.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...

pipsyl chloride C6H4ClO2S[3, 64]



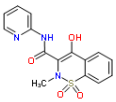
Compound Data

Melting point	**83.50 °C**	**356.65 K**			
CSID	7121	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	302.5172	**H bond donors**	0	**ACD/LogP**	3.28
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	2.04 g/cm^3
SMILES	O=S(Cl)(=O)c1ccc(I)cc1				
STD InChIKey	POXFXTSTVWDWIR-UHFFFAOYAO				

Melting Points

mp °C	source
82.00	Alfa Aesar
85.00	PHYSPROP

piroxicam C15H13N3O4S[9, 35, 44, 64]



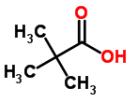
Compound Data

Melting point	**199.07 °C**	**472.22 K**			
CSID	10442653	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	331.3464	**H bond donors**	2	**ACD/LogP**	1.57
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.56 g/cm^3
SMILES	OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3				
STD InChIKey	QYSPLQLAKJAUJT-UHFFFAOYAT				

Melting Points

mp °C	source
198.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
199.00	EPISuite-ChemSpider
200.30	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
199.00	PHYSPROP

pivalic acid C5H10O2[3, 4, 64]



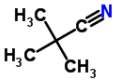
Compound Data

Melting point	**34.83 °C**	**307.98 K**			
CSID	6177	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	1	**ACD/LogP**	0.94
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.96 g/cm^3
SMILES	O=C(O)C(C)(C)C				
STD InChIKey	IUGYQRQAERSCNH-UHFFFAOYAP				

Melting Points

mp °C	source
33.00	Alfa Aesar
36.00	American Petroleum Institute. Research Project 44; Selected ...
35.50	PHYSPROP

pivalonitrile C5H9N[3, 64]



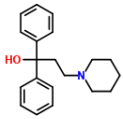
Compound Data

Melting point	**16.00 °C**	**289.15 K**			
CSID	11909	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	83.1317	**H bond donors**	0	**ACD/LogP**	0.78
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.80 g/cm^3
SMILES	N#CC(C)(C)C				
STD InChIKey	JAMNHZBIQDNHMM-UHFFFAOYAT				

Melting Points

mp °C	source
17.00	Alfa Aesar
15.00	PHYSPROP

pridinol C20H25NO[9, 48, 64]



Compound Data

Melting point	**120.17 °C**	**393.32 K**			
CSID	4735	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	295.4186	**H bond donors**	1	**ACD/LogP**	3.84
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.08 g/cm^3
SMILES	OC(c1ccccc1)(c2ccccc2)CCN3CCCCC3				
STD InChIKey	RQXCLMGKHJWMOA-UHFFFAOYAW				

Melting Points

mp °C	source
120.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
120.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
120.50	PHYSPROP

primidone C12H14N2O2[9, 32, 44, 64]

Compound Data

Melting point	**281.38 °C**	**554.52 K**			
CSID	4740	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	218.2518	**H bond donors**	2	**ACD/LogP**	0.40
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.14 g/cm^3
SMILES	O=C1NCNC(=O)C1(c2ccccc2)CC				
STD InChIKey	DQMZLTXERSFNPB-UHFFFAOYAX				

Melting Points

mp °C	source
281.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
281.50	DrugBank
281.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
281.50	PHYSPROP

probarbital C9H14N2O3[35, 44, 64]

Compound Data

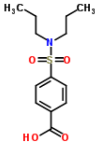
Melting point	**201.33 °C**	**474.48 K**			
CSID	6213	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	198.2191	**H bond donors**	2	**ACD/LogP**	0.99
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.12 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(C(C)C)CC				
STD InChIKey	HHLXJTDUHFBYAU-UHFFFAOYAJ				

Melting Points

mp °C	source
203.00	EPISuite-ChemSpider
198.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
203.00	PHYSPROP

probenecid C13H19NO4S[3, 9, 32, 44, 61, 64]

Compound Data



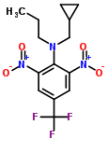
Melting point	**196.75 °C**	**469.90 K**			
CSID	4742	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	285.3593	**H bond donors**	1	**ACD/LogP**	3.30
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.22 g/cm^3
SMILES	O=S(=O)(N(CCC)CCC)c1ccc(C(=O)O)cc1				
STD InChIKey	DBABZHXKTCFAPX-UHFFFAOYAR				

Melting Points

mp °C	source
199.00	Alfa Aesar
198.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
195.00	DrugBank
198.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
195.00	Oxford University MSDS
195.00	PHYSPROP

profluralin C14H16F3N3O4[64, 70]

Compound Data



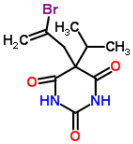
Melting point	**32.15 °C**	**305.30 K**			
CSID	30913	**H bond acceptors**	7	**Rule of 5 violations**	1
Molecular weight	347.2897	**H bond donors**	0	**ACD/LogP**	5.25
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.41 g/cm^3
SMILES	[O-][N+](=O)c2c(N(CCC)CC1CC1)c([N+]([O-])=O)cc(c2)C(F)(F)F				
STD InChIKey	ITVQAKZNYJEWKS-UHFFFAOYAO				

Melting Points

mp °C	source
32.30	PHYSPROP
32.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

propallylonal C10H13BrN2O3[9, 48, 64]

Compound Data



Melting point	**178.33 °C**	**451.48 K**			
CSID	10554	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	289.1258	**H bond donors**	2	**ACD/LogP**	2.03
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.44 g/cm^3
SMILES	O=C1NC(=O)NC(=O)C1(C(C)C)CC(\Br)=C				
STD InChIKey	KTGWBBOJAGDSHN-UHFFFAOYAO				

Melting Points

mp °C	source

177.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
177.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
181.00	PHYSPROP

propane C3H8[61, 64, 73]

Compound Data

Melting point	**-187.75 °C**	**85.40 K**			
CSID	6094	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	44.0956	**H bond donors**	0	**ACD/LogP**	2.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.56 g/cm^3
SMILES	CCC				
STD InChIKey	ATUOYWHBWRKTHZ-UHFFFAOYAU				

Melting Points

mp °C	source
-188.00	Oxford University MSDS
-187.60	PHYSPROP
-187.65	Streng AG Journal of Chemical and Engineering Data 16(3) 357...

propane sultone C3H6O3S[3, 61, 64]

Compound Data

Melting point	**31.83 °C**	**304.98 K**			
CSID	13626	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	122.1429	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.42 g/cm^3
SMILES	C1COS(=O)(=O)C1				
STD InChIKey	FSSPGSAQUIYDCN-UHFFFAOYAH				

Melting Points

mp °C	source
32.00	Alfa Aesar
32.00	Oxford University MSDS
31.50	PHYSPROP

propene C3H6[60, 61, 64, 73]

Compound Data

Melting point	**-185.09 °C**	**88.06 K**			
CSID	7954	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	42.0797	**H bond donors**	0	**ACD/LogP**	1.83
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.57 g/cm^3
SMILES	CC=C				
STD InChIKey	QQONPFPTGQHPMA-UHFFFAOYAA				

Melting Points

mp °C	source
-185.20	Oka T; Sato S. Bulletin of the Chemical Society of Japan 42(...
-185.00	Oxford University MSDS
-185.00	PHYSPROP
-185.15	Streng AG Journal of Chemical and Engineering Data 16(3) 357...

propionaldehyde C3H6O[3, 4, 61, 64]

Compound Data

Melting point	**-80.50 °C**	**192.65 K**			
CSID	512	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	58.0791	**H bond donors**	0	**ACD/LogP**	0.40
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.77 g/cm^3
SMILES	CCC=O				

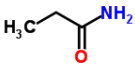
STD InChIKey	NBBJYMSMWIIQGU-UHFFFAOYAZ

Melting Points

mp °C	source
-81.00	Alfa Aesar
-80.00	American Petroleum Institute. Research Project 44; Selected ...
-81.00	Oxford University MSDS
-80.00	PHYSPROP

propionamide C3H7NO[3, 64]

Compound Data



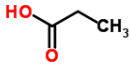
Melting point	**79.65 °C**	**352.80 K**				
CSID	6330	**H bond acceptors**	2	**Rule of 5 violations**	0	
Molecular weight	73.0938	**H bond donors**	2	**ACD/LogP**	-0.70	
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.93 g/cm^3	
SMILES	O=C(N)CC					
STD InChIKey	QLNJFJADRCOGBJ-UHFFFAOYAE					

Melting Points

mp °C	source
78.00	Alfa Aesar
81.30	PHYSPROP

propionic acid C3H6O2[3, 4, 35, 61, 64]

Compound Data



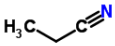
Melting point	**-20.92 °C**	**252.23 K**				
CSID	1005	**H bond acceptors**	2	**Rule of 5 violations**	0	
Molecular weight	74.0785	**H bond donors**	1	**ACD/LogP**	0.19	
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.02 g/cm^3	
SMILES	CCC(=O)O					
STD InChIKey	XBDQKXXYIPTUBI-UHFFFAOYAP					

Melting Points

mp °C	source
-21.00	Alfa Aesar
-21.00	American Petroleum Institute. Research Project 44; Selected ...
-20.70	EPISuite-ChemSpider
-20.80	Oxford University MSDS
-21.10	PHYSPROP

propiononitrile C3H5N[2, 3, 31, 61, 64]

Compound Data



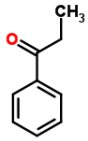
Melting point	**-92.56 °C**	**180.59 K**				
CSID	7566	**H bond acceptors**	1	**Rule of 5 violations**	0	
Molecular weight	55.0785	**H bond donors**	0	**ACD/LogP**	0.18	
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.77 g/cm^3	
SMILES	CCC#N					
STD InChIKey	FVSKHRXBFJPNKK-UHFFFAOYAD					

Melting Points

mp °C	source
-93.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-92.00	Alfa Aesar
-93.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-92.00	Oxford University MSDS
-92.80	PHYSPROP

propiophenone C9H10O[3, 31, 61, 64]

Compound Data



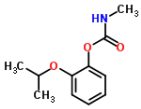
Melting point	**18.40 °C**	**291.55 K**			
CSID	6881	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	134.1751	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.98 g/cm^3
SMILES	CCC(=O)c1ccccc1				
STD InChIKey	KRIOVPPHQSLHCZ-UHFFFAOYAT				

Melting Points

mp °C	source
18.00	Alfa Aesar
19.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
18.00	Oxford University MSDS
18.60	PHYSPROP

propoxur C11H15NO3[44, 64]

Compound Data



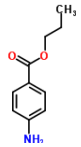
Melting point	**90.75 °C**	**363.90 K**			
CSID	4775	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	209.2417	**H bond donors**	1	**ACD/LogP**	1.60
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.08 g/cm^3
SMILES	O=C(Oc1ccccc1OC(C)C)NC				
STD InChIKey	ISRUGXGCCGIOQO-UHFFFAOYAH				

Melting Points

mp °C	source
91.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
90.00	PHYSPROP

propyl 4-aminobenzoate C10H13NO2[3, 64]

Compound Data



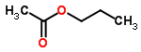
Melting point	**74.50 °C**	**347.65 K**			
CSID	6906	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	179.2157	**H bond donors**	2	**ACD/LogP**	2.48
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.10 g/cm^3
SMILES	O=C(OCCC)c1ccc(N)cc1				
STD InChIKey	NBFQYHKHPBMJJV-UHFFFAOYAX				

Melting Points

mp °C	source
74.00	Alfa Aesar
75.00	PHYSPROP

propyl acetate C5H10O2[2, 3, 32, 61, 64]

Compound Data

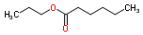


Melting point	**-93.60 °C**	**179.55 K**			
CSID	7706	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	0	**ACD/LogP**	1.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.89 g/cm^3
SMILES	O=C(OCCC)C				
STD InChIKey	YKYONYBAUNKHLG-UHFFFAOYAC				

Melting Points

mp °C	source
-95.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-92.00	Alfa Aesar
-93.00	DrugBank
-95.00	Oxford University MSDS
-93.00	PHYSPROP

propyl hexanoate C9H18O2[3, 64]



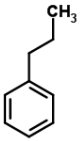
Compound Data

Melting point	**-68.85 °C**	**204.30 K**			
CSID	11790	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	158.238	**H bond donors**	0	**ACD/LogP**	3.37
Phase 25 °C	liquid/gas	**Rotatable bonds**	7	**Predicted density**	0.88 g/cm^3
SMILES	O=C(OCCC)CCCCC				
STD InChIKey	HTUIWRWYYVBCFT-UHFFFAOYAY				

Melting Points

mp °C	source
-69.00	Alfa Aesar
-68.70	PHYSPROP

propylbenzene C9H12[3, 4, 61, 64]



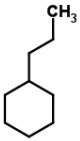
Compound Data

Melting point	**-99.62 °C**	**173.52 K**			
CSID	7385	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	120.1916	**H bond donors**	0	**ACD/LogP**	3.74
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.87 g/cm^3
SMILES	c1ccccc1CCC				
STD InChIKey	ODLMAHJVESYWTB-UHFFFAOYAK				

Melting Points

mp °C	source
-100.00	Alfa Aesar
-100.00	American Petroleum Institute. Research Project 44; Selected ...
-99.00	Oxford University MSDS
-99.50	PHYSPROP

propylcyclohexane C9H18[4, 64]



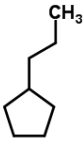
Compound Data

Melting point	**-94.95 °C**	**178.20 K**			
CSID	14752	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	126.2392	**H bond donors**	0	**ACD/LogP**	4.94
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.79 g/cm^3
SMILES	CCCC1CCCCC1				
STD InChIKey	DEDZSLCZHWTGOR-UHFFFAOYAV				

Melting Points

mp °C	source
-95.00	American Petroleum Institute. Research Project 44; Selected ...
-94.90	PHYSPROP

propylcyclopentane C8H16[4, 64]



Compound Data

Melting point	**-117.15 °C**	**156.00 K**			
CSID	15438	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	112.2126	**H bond donors**	0	**ACD/LogP**	4.38
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.79 g/cm^3
SMILES	CCCC1CCCC1				
STD InChIKey	KDIAMAVWIJYWHN-UHFFFAOYAU				

Melting Points

mp °C	source
-117.00	American Petroleum Institute. Research Project 44; Selected ...
-117.30	PHYSPROP

propylene oxide C3H6O[3, 61, 64]

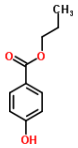
Compound Data

Melting point	**-111.97 °C**	**161.18 K**			
CSID	6138	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	58.0791	**H bond donors**	0	**ACD/LogP**	0.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.90 g/cm^3
SMILES	CC1CO1				
STD InChIKey	GOOHAUXETOMSMM-UHFFFAOYAI				

Melting Points

mp °C	source
-112.00	Alfa Aesar
-112.00	Oxford University MSDS
-111.90	PHYSPROP

propylparaben C10H12O3[3, 28, 35, 44, 56, 61, 64, 70, 72, 72]



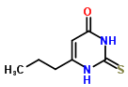
Compound Data

Melting point	**96.60 °C**	**369.75 K**			
CSID	6907	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	180.2005	**H bond donors**	1	**ACD/LogP**	2.93
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.13 g/cm^3
SMILES	O=C(OCCC)c1ccc(O)cc1				
STD InChIKey	QELSKZZBTMNZEB-UHFFFAOYAD				

Melting Points

mp °C	source
97.00	Alfa Aesar
97.00	CRC Handbook of Chemistry and Physics
97.00	EPISuite-ChemSpider
96.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
96.50	Merck Index
96.50	Oxford University MSDS
97.00	PHYSPROP
96.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
96.00	Sigma-Aldrich
96.50	Sigma-Aldrich

propylthiouracil C7H10N2OS[32, 61, 64]



Compound Data

Melting point	**219.67 °C**	**492.82 K**			
CSID	571424	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	170.2321	**H bond donors**	2	**ACD/LogP**	1.37
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.24 g/cm^3
SMILES	S=C1N/C(=C\C(=O)N1)CCC				
STD InChIKey	KNAHARQHSZJURB-UHFFFAOYAR				

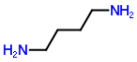
Melting Points

mp °C	source
219.00	DrugBank
220.00	Oxford University MSDS
220.00	PHYSPROP

putrescine C4H12N2[3, 32, 61, 64]

Compound Data

Melting point	**27.38 °C**	**300.52 K**			
CSID	13837702	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	88.1515	**H bond donors**	4	**ACD/LogP**	0.00



Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	0.86 g/cm^3
SMILES	C(CCN)CN				
STD InChIKey	KIDHWZJUCRJVML-UHFFFAOYAX				

Melting Points

mp °C	source
27.00	Alfa Aesar
27.50	DrugBank
27.50	Oxford University MSDS
27.50	PHYSPROP

pyrazinamide C5H5N3O[9, 32, 44, 48, 64]

Compound Data

Melting point	**190.40 °C**	**463.55 K**			
CSID	1017	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	123.1127	**H bond donors**	2	**ACD/LogP**	-0.37
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	O=C(N)c1nccnc1				
STD InChIKey	IPEHBUMCGVEMRF-UHFFFAOYAZ				

Melting Points

mp °C	source
189.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
192.00	DrugBank
190.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
189.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
192.00	PHYSPROP

pyrazine C4H4N2[3, 61, 64]

Compound Data

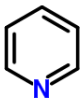
Melting point	**54.33 °C**	**327.48 K**			
CSID	8904	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	80.088	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	c1cnccn1				
STD InChIKey	KYQCOXFCLRTKLS-UHFFFAOYAV				

Melting Points

mp °C	source
53.00	Alfa Aesar
55.00	Oxford University MSDS
55.00	PHYSPROP

pyridine C5H5N[2, 3, 61, 64]

Compound Data



Melting point	**-41.90 °C**	**231.25 K**			
CSID	1020	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	79.0999	**H bond donors**	0	**ACD/LogP**	0.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.96 g/cm^3
SMILES	c1ccncc1				
STD InChIKey	JUJWROOIHBZHMG-UHFFFAOYAY				

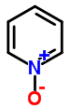
Melting Points

mp °C	source
-42.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-42.00	Alfa Aesar

-42.00	Oxford University MSDS
-41.60	PHYSPROP

pyridine N-oxide C5H5NO[3, 64]

Compound Data



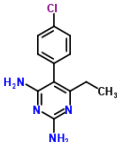
Melting point	**64.75 °C**	**337.90 K**			
CSID	12229	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	95.0993	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.03 g/cm^3
SMILES	c1cc[n+](cc1)[O-]				
STD InChIKey	ILVXOBCQQYKLDS-UHFFFAOYAZ				

Melting Points

mp °C	source
64.00	Alfa Aesar
65.50	PHYSPROP

pyrimethamine C12H13ClN4[32, 61, 64]

Compound Data



Melting point	**233.33 °C**	**506.48 K**			
CSID	4819	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	248.7114	**H bond donors**	4	**ACD/LogP**	2.75
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.30 g/cm^3
SMILES	Clc2ccc(c1c(nc(nc1CC)N)N)cc2				
STD InChIKey	WKSAUQYGYAYLPV-UHFFFAOYAW				

Melting Points

mp °C	source
233.50	DrugBank
233.00	Oxford University MSDS
233.50	PHYSPROP

pyrimidine C4H4N2[3, 61, 64]

Compound Data

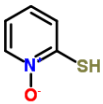
Melting point	**21.33 °C**	**294.48 K**			
CSID	8903	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	80.088	**H bond donors**	0	**ACD/LogP**	0.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.05 g/cm^3
SMILES	c1cncnc1				
STD InChIKey	CZPWVGJYEJSRLH-UHFFFAOYAT				

Melting Points

mp °C	source
21.00	Alfa Aesar
21.00	Oxford University MSDS
22.00	PHYSPROP

pyrithione C5H5NOS[3, 61]

Compound Data



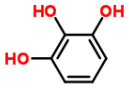
Melting point	**70.75 °C**	**343.90 K**			
CSID	10446934	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	127.1643	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	[O-][n+]1ccccc1S				
STD InChIKey	FGVVTMRZYROCTH-UHFFFAOYAC				

Melting Points

mp °C	source

71.00	Alfa Aesar
70.50	Oxford University MSDS

pyrogallol C6H6O3[2, 3, 61, 64]



Compound Data

Melting point	**133.00 °C**	**406.15 K**			
CSID	13835557	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	126.11	**H bond donors**	3	**ACD/LogP**	0.29
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.49 g/cm^3
SMILES	Oc1cccc(O)c1O				
STD InChIKey	WQGWDDDVZFFDIG-UHFFFAOYAT				

Melting Points

mp °C	source
134.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
133.00	Alfa Aesar
132.00	Oxford University MSDS
133.00	PHYSPROP

pyrrole C4H5N[61, 64]

Compound Data

Melting point	**-23.20 °C**	**249.95 K**			
CSID	7736	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	67.0892	**H bond donors**	1	**ACD/LogP**	0.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.99 g/cm^3
SMILES	c1cc[nH]c1				
STD InChIKey	KAESVJOAVNADME-UHFFFAOYAK				

Melting Points

mp °C	source
-23.00	Oxford University MSDS
-23.40	PHYSPROP

pyrrole-2-carboxaldehyde C5H5NO[3, 64]

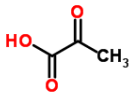
Compound Data

Melting point	**44.75 °C**	**317.90 K**			
CSID	13254	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	95.0993	**H bond donors**	1	**ACD/LogP**	0.64
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.20 g/cm^3
SMILES	O=Cc1cccn1				
STD InChIKey	ZSKGQVFRTSEPJT-UHFFFAOYAN				

Melting Points

mp °C	source
43.00	Alfa Aesar
46.50	PHYSPROP

pyruvic acid C3H4O3[3, 3, 6, 28, 32, 61, 61, 64, 72]



Compound Data

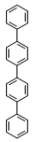
Melting point	**12.16 °C**	**285.31 K**			
CSID	1031	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	88.0621	**H bond donors**	1	**ACD/LogP**	-1.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	1.26 g/cm^3
SMILES	O=C(C(=O)O)C				
STD InChIKey	LCTONWCANYUPML-UHFFFAOYAJ				

Melting Points

mp °C	source

11.00	Alfa Aesar
11.50	Alfa Aesar
12.00	Bedoukian Research
13.80	CRC Handbook of Chemistry and Physics
11.80	DrugBank
12.00	Oxford University MSDS
12.00	Oxford University MSDS
13.80	PHYSPROP
11.50	Sigma-Aldrich

quaterphenyl C24H18[3, 64]



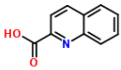
Compound Data

Melting point	**318.50 °C**	**591.65 K**			
CSID	8353	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	306.3997	**H bond donors**	0	**ACD/LogP**	7.29
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.07 g/cm^3
SMILES	c1cc(ccc1c2ccccc2)c3ccc(cc3)c4ccccc4				
STD InChIKey	GPRIERYVMZVKTC-UHFFFAOYAG				

Melting Points

mp °C	source
317.00	Alfa Aesar
320.00	PHYSPROP

quinaldic acid C10H7NO2[3, 32, 64]



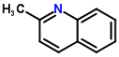
Compound Data

Melting point	**156.67 °C**	**429.82 K**			
CSID	6857	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	173.1681	**H bond donors**	1	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	c1ccc2c(c1)ccc(n2)C(=O)O				
STD InChIKey	LOAUVZALPPNFOQ-UHFFFAOYAV				

Melting Points

mp °C	source
158.00	Alfa Aesar
156.00	DrugBank
156.00	PHYSPROP

quinaldine C10H9N[3, 64]



Compound Data

Melting point	**-1.75 °C**	**271.40 K**			
CSID	13870160	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.1852	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.08 g/cm^3
SMILES	Cc1ccc2ccccc2n1				
STD InChIKey	SMUQFGGVLNAIOZ-UHFFFAOYAY				

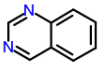
Melting Points

mp °C	source
-2.00	Alfa Aesar
-1.50	PHYSPROP

quinazoline C8H6N2[3, 64]

Compound Data

Melting point	**47.50 °C**	**320.65 K**			
CSID	8855	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1466	**H bond donors**	0	**ACD/LogP**	1.00



Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.18 g/cm^3
SMILES	c1ccc2c(c1)cncn2				
STD InChIKey	JWVCLYRUEFBMGU-UHFFFAOYAV				

Melting Points

mp °C	source
47.00	Alfa Aesar
48.00	PHYSPROP

quinoline C9H7N[3, 64]

Compound Data

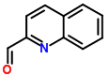
Melting point	**-14.89 °C**	**258.26 K**			
CSID	6780	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	129.1586	**H bond donors**	0	**ACD/LogP**	2.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.11 g/cm^3
SMILES	n1cccc2ccccc12				
STD InChIKey	SMWDFEZZVXVKRB-UHFFFAOYAU				

Melting Points

mp °C	source
-15.00	Alfa Aesar
-14.78	PHYSPROP

quinoline-2-carboxaldehyde C10H7NO[3, 64]

Compound Data



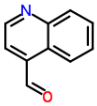
Melting point	**69.50 °C**	**342.65 K**			
CSID	71926	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	157.1687	**H bond donors**	0	**ACD/LogP**	2.14
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	O=Cc1nc2ccccc2cc1				
STD InChIKey	WPYJKGWLDJECQD-UHFFFAOYAZ				

Melting Points

mp °C	source
68.00	Alfa Aesar
71.00	PHYSPROP

quinoline-4-carboxaldehyde C10H7NO[3, 64]

Compound Data



Melting point	**50.50 °C**	**323.65 K**			
CSID	70450	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	157.1687	**H bond donors**	0	**ACD/LogP**	1.51
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.22 g/cm^3
SMILES	O=Cc1c2ccccc2ncc1				
STD InChIKey	MGCGJBXTNWUHQE-UHFFFAOYAT				

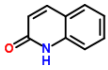
Melting Points

mp °C	source
50.00	Alfa Aesar
51.00	PHYSPROP

quinolone C9H7NO[3, 64]

Compound Data

Melting point	**198.75 °C**	**471.90 K**			
CSID	5816	**H bond acceptors**	2	**Rule of 5 violations**	0



Molecular weight	145.158	**H bond donors**	1	**ACD/LogP**	1.26
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	O=C2/C=C\c1c(cccc1)N2				
STD InChIKey	LISFMEBWQUVKPJ-UHFFFAOYAF				

Melting Points

mp °C	source
198.00	Alfa Aesar
199.50	PHYSPROP

quinoxaline C8H6N2[3, 64]

Compound Data

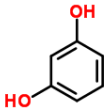
Melting point	**29.00 °C**	**302.15 K**			
CSID	21106470	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	130.1466	**H bond donors**	0	**ACD/LogP**	1.30
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.18 g/cm^3
SMILES	c1cccc2nccnc12				
STD InChIKey	XSCHRSMBECNVNS-UHFFFAOYAS				

Melting Points

mp °C	source
30.00	Alfa Aesar
28.00	PHYSPROP

resorcinol C6H6O2[2, 3, 61, 64]

Compound Data



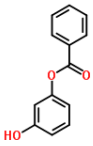
Melting point	**110.75 °C**	**383.90 K**			
CSID	4878	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	110.1106	**H bond donors**	2	**ACD/LogP**	0.82
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.28 g/cm^3
SMILES	c1cc(cc(c1)O)O				
STD InChIKey	GHMLBKRAJCXXBS-UHFFFAOYAB				

Melting Points

mp °C	source
110.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
111.00	Alfa Aesar
111.00	Oxford University MSDS
111.00	PHYSPROP

resorcinol monobenzoate C13H10O3[3, 64]

Compound Data



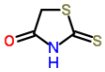
Melting point	**133.00 °C**	**406.15 K**			
CSID	8366	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	214.2167	**H bond donors**	1	**ACD/LogP**	3.03
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.25 g/cm^3
SMILES	O=C(Oc1cccc(O)c1)c2ccccc2				
STD InChIKey	GDESWOTWNNGOMW-UHFFFAOYAL				

Melting Points

mp °C	source
132.00	Alfa Aesar
134.00	PHYSPROP

rhodanine C3H3NOS2[3, 64]

Compound Data



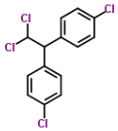
Melting point	**169.50 °C**	**442.65 K**			
CSID	1013337	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	133.192	**H bond donors**	1	**ACD/LogP**	0.06
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.59 g/cm^3
SMILES	O=C1NC(=S)SC1				
STD InChIKey	KIWUVOGUEXMXSV-UHFFFAOYAP				

Melting Points

mp °C	source
169.00	Alfa Aesar
170.00	PHYSPROP

rothane C14H10Cl4[61, 64]

Compound Data



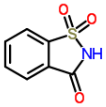
Melting point	**109.25 °C**	**382.40 K**			
CSID	6057	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	320.0412	**H bond donors**	0	**ACD/LogP**	5.39
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.37 g/cm^3
SMILES	Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)Cl				
STD InChIKey	AHJKRLASYNVKDZ-UHFFFAOYAJ				

Melting Points

mp °C	source
109.00	Oxford University MSDS
109.50	PHYSPROP

saccharin C7H5NO3S[3, 44]

Compound Data



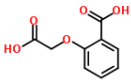
Melting point	**229.15 °C**	**502.30 K**			
CSID	4959	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	183.1845	**H bond donors**	1	**ACD/LogP**	0.91
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.56 g/cm^3
SMILES	O=C2c1ccccc1S(=O)(=O)N2				
STD InChIKey	CVHZOJJKTDOEJC-UHFFFAOYAR				

Melting Points

mp °C	source
229.00	Alfa Aesar
229.30	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...

salicylacetic acid C9H8O5[3, 64]

Compound Data



Melting point	**190.00 °C**	**463.15 K**			
CSID	62668	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	196.1568	**H bond donors**	2	**ACD/LogP**	0.70
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.43 g/cm^3
SMILES	O=C(O)c1ccccc1OCC(=O)O				
STD InChIKey	JLLXSRLEXBECPY-UHFFFAOYAI				

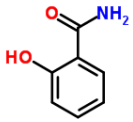
Melting Points

mp °C	source
189.00	Alfa Aesar
191.00	PHYSPROP

salicylamide C7H7NO2[2, 3, 35, 44, 61, 64]

Compound Data

Melting point	**141.00 °C**	**414.15 K**			
CSID	4963	**H bond acceptors**	3	**Rule of 5 violations**	0



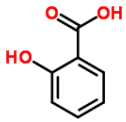
Molecular weight	137.136	**H bond donors**	3	**ACD/LogP**	1.41
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.29 g/cm^3
SMILES	O=C(c1ccccc1O)N				
STD InChIKey	SKZKKFZAGNVIMN-UHFFFAOYAB				

Melting Points

mp °C	source
142.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
140.00	Alfa Aesar
142.00	EPISuite-ChemSpider
140.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
140.00	Oxford University MSDS
142.00	PHYSPROP

salicylic acid C7H6O3[2, 3, 9, 20, 21, 32, 35, 44, 48, 61, 61, 64, 70, 84]

Compound Data



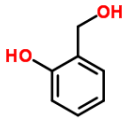
Melting point	**158.75 °C 431.90 K**				
CSID	331	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	138.1207	**H bond donors**	2	**ACD/LogP**	2.01
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.38 g/cm^3
SMILES	c1ccc(c(c1)C(=O)O)O				
STD InChIKey	YGSDEFSMJLZEOE-UHFFFAOYAQ				

Melting Points

mp °C	source
160.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
159.00	Alfa Aesar
157.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
159.00	Chemical Land
158.00	ChemIDplus
158.00	DrugBank
158.00	EPISuite-ChemSpider
158.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
157.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
161.00	Oxford University MSDS
161.00	Oxford University MSDS
159.00	PHYSPROP
158.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)
159.50	Wolfram Alpha

salicylic alcohol C7H8O2[2, 3, 64]

Compound Data

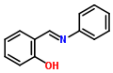


Melting point	**85.67 °C 358.82 K**				
CSID	4962	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	124.1372	**H bond donors**	2	**ACD/LogP**	0.30
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	OCc1ccccc1O				
STD InChIKey	CQRYARSYNCAZFO-UHFFFAOYAM				

Melting Points

mp °C	source
85.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
85.00	Alfa Aesar
87.00	PHYSPROP

salicylideneaniline C13H11NO[64, 77]



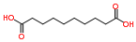
Compound Data

Melting point	**48.50 °C**	**321.65 K**			
CSID	10237273	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	197.2325	**H bond donors**	1	**ACD/LogP**	3.09
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.06 g/cm^3
SMILES	Oc2ccccc2/C=N/c1ccccc1				
STD InChIKey	QIYHCQVVYSSDTI-GXDHUFHOBW				

Melting Points

mp °C	source
49.50	PHYSPROP
47.50	UsefulChem EXP269

sebacic acid C10H18O4[2, 3, 61, 64]



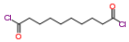
Compound Data

Melting point	**132.82 °C**	**405.97 K**			
CSID	5004	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	202.2475	**H bond donors**	2	**ACD/LogP**	1.86
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.11 g/cm^3
SMILES	O=C(O)CCCCCCCCC(=O)O				
STD InChIKey	CXMXRPHRNRROMY-UHFFFAOYAE				

Melting Points

mp °C	source
133.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
133.00	Alfa Aesar
134.50	Oxford University MSDS
130.80	PHYSPROP

sebacoyl chloride C10H16Cl2O2[3, 64]



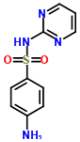
Compound Data

Melting point	**-3.75 °C**	**269.40 K**			
CSID	59462	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	239.1388	**H bond donors**	0	**ACD/LogP**	3.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	1.14 g/cm^3
SMILES	ClC(=O)CCCCCCCCC(Cl)=O				
STD InChIKey	WMPOZLHMGVKUEJ-UHFFFAOYAH				

Melting Points

mp °C	source
-5.00	Alfa Aesar
-2.50	PHYSPROP

silvadene C10H10N4O2S[3, 35, 44]



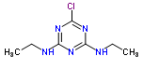
Compound Data

Melting point	**254.33 °C**	**527.48 K**			
CSID	5026	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	250.277	**H bond donors**	3	**ACD/LogP**	-0.12
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.50 g/cm^3
SMILES	O=S(=O)(Nc1nccn1)c2ccc(N)cc2				
STD InChIKey	SEEPANYCNGTZFQ-UHFFFAOYAL				

Melting Points

mp °C	source
255.00	Alfa Aesar
255.50	EPISuite-ChemSpider
252.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...

simazine C7H12ClN5[3, 64]



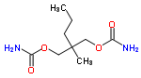
Compound Data

Melting point	**227.00 °C**	**500.15 K**			
CSID	5027	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	201.6567	**H bond donors**	2	**ACD/LogP**	2.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	Clc1nc(nc(n1)NCC)NCC				
STD InChIKey	ODCWYMIRDDJXKW-UHFFFAOYAN				

Melting Points

mp °C	source
228.00	Alfa Aesar
226.00	PHYSPROP

sowell C9H18N2O4[9, 32, 44, 48, 61, 64]



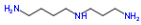
Compound Data

Melting point	**104.67 °C**	**377.82 K**			
CSID	3924	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	218.2502	**H bond donors**	4	**ACD/LogP**	0.70
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.14 g/cm^3
SMILES	O=C(OCC(COC(=O)N)(C)CCC)N				
STD InChIKey	NPPQSCRMBWNHMW-UHFFFAOYAM				

Melting Points

mp °C	source
104.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
105.00	DrugBank
105.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
104.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
105.00	Oxford University MSDS
105.00	PHYSPROP

spermidine C7H19N3[3, 61, 64]



Compound Data

Melting point	**23.75 °C**	**296.90 K**			
CSID	1071	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	145.2459	**H bond donors**	5	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.91 g/cm^3
SMILES	C(CCNCCCN)CN				
STD InChIKey	ATHGHQPFGPMSJY-UHFFFAOYAK				

Melting Points

mp °C	source
24.00	Alfa Aesar
23.50	Oxford University MSDS
	Values not used in calculating the average melting point
258.00	PHYSPROP[1]

1. salt JCB

spermine C10H26N4[3, 32, 64, 64]

Compound Data

Melting point	**28.67 °C**	**301.82 K**			
CSID	1072	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	202.3402	**H bond donors**	6	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	13	**Predicted density**	0.93 g/cm^3
SMILES	C(CCNCCCN)CNCCCN				
STD InChIKey	PFNFFQXMRSDOHW-UHFFFAOYAC				

Melting Points

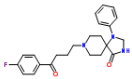
mp °C	source

29.00	Alfa Aesar
28.00	DrugBank
29.00	PHYSPROP
	Values not used in calculating the average melting point
301.50	PHYSPROP[1]

1. salt JCB

spiperone C23H26FN3O2[9, 48, 64]

Compound Data



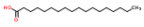
Melting point	**190.60 °C**	**463.75 K**			
CSID	5075	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	395.4698	**H bond donors**	1	**ACD/LogP**	3.25
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.27 g/cm^3
SMILES	c1ccc(cc1)N2CNC(=O)C23CCN(CC3)CCCC(=O)c4ccc(cc4)F				
STD InChIKey	DKGZKTPJOSAWFA-UHFFFAOYAX				

Melting Points

mp °C	source
190.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
190.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
191.80	PHYSPROP

stearic acid C18H36O2[3, 61, 64]

Compound Data



Melting point	**69.43 °C**	**342.58 K**			
CSID	5091	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	284.4772	**H bond donors**	1	**ACD/LogP**	8.22
Phase 25 °C	solid	**Rotatable bonds**	16	**Predicted density**	0.89 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCCCCCCC				
STD InChIKey	QIQXTHQIDYTFRH-UHFFFAOYAB				

Melting Points

mp °C	source
71.00	Alfa Aesar
68.00	Oxford University MSDS
69.30	PHYSPROP

stearone C35H70O[3, 64]

Compound Data

Melting point	**88.00 °C**	**361.15 K**			
CSID	10009	**H bond acceptors**	1	**Rule of 5 violations**	2
Molecular weight	506.9297	**H bond donors**	0	**ACD/LogP**	16.85
Phase 25 °C	solid	**Rotatable bonds**	32	**Predicted density**	0.84 g/cm^3
SMILES	O=C(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC				
STD InChIKey	DMCJFWXGXUEHFD-UHFFFAOYAX				

Melting Points

mp °C	source
87.00	Alfa Aesar
89.00	PHYSPROP

stearylamine C18H39N[35, 61, 64]

Compound Data

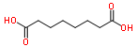
Melting point	**53.93 °C**	**327.08 K**			
CSID	15016	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	269.509	**H bond donors**	2	**ACD/LogP**	8.19
Phase 25 °C	solid	**Rotatable bonds**	17	**Predicted density**	0.82 g/cm^3

SMILES	CCCCCCCCCCCCCCCCCCN
STD InChIKey	REYJJPSVUYRZGE-UHFFFAOYAC

Melting Points

mp °C	source
52.90	EPISuite-ChemSpider
56.00	Oxford University MSDS
52.90	PHYSPROP

suberic acid C8H14O4[2, 3, 61, 64]



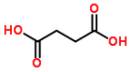
Compound Data

Melting point	**143.50 °C**	**416.65 K**			
CSID	10025	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	174.1944	**H bond donors**	2	**ACD/LogP**	0.80
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.16 g/cm^3
SMILES	O=C(O)CCCCCCC(=O)O				
STD InChIKey	TYFQFVWCELRYAO-UHFFFAOYAN				

Melting Points

mp °C	source
144.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
143.00	Alfa Aesar
143.00	Oxford University MSDS
144.00	PHYSPROP

succinic acid C4H6O4[2, 3, 32, 35, 61, 64]



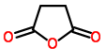
Compound Data

Melting point	**187.08 °C**	**460.23 K**			
CSID	1078	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	118.088	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.41 g/cm^3
SMILES	C(CC(=O)O)C(=O)O				
STD InChIKey	KDYFGRWQOYBRFD-UHFFFAOYAC				

Melting Points

mp °C	source
188.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
187.00	Alfa Aesar
186.50	DrugBank
188.00	EPISuite-ChemSpider
185.00	Oxford University MSDS
188.00	PHYSPROP

succinic anhydride C4H4O3[3, 61, 64]



Compound Data

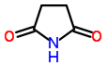
Melting point	**119.50 °C**	**392.65 K**			
CSID	7634	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	100.0728	**H bond donors**	0	**ACD/LogP**	-1.30
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.38 g/cm^3
SMILES	O=C1OC(=O)CC1				
STD InChIKey	RINCXYDBBGOEEQ-UHFFFAOYAN				

Melting Points

mp °C	source
120.00	Alfa Aesar

119.50	Oxford University MSDS
119.00	PHYSPROP

succinimide C4H5NO2[3, 64]



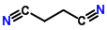
Compound Data

Melting point	**125.25 °C**	**398.40 K**			
CSID	10955	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	99.088	**H bond donors**	1	**ACD/LogP**	-1.18
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	O=C1NC(=O)CC1				
STD InChIKey	KZNICNPSHKQLFF-UHFFFAOYAV				

Melting Points

mp °C	source
124.00	Alfa Aesar
126.50	PHYSPROP

succinonitrile C4H4N2[2, 3, 64]



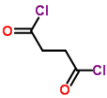
Compound Data

Melting point	**54.83 °C**	**327.98 K**			
CSID	21106481	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	80.088	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3
SMILES	N#CCCC#N				
STD InChIKey	IAHFWCOBPZCAEA-UHFFFAOYAW				

Melting Points

mp °C	source
56.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
54.50	PHYSPROP

succinyl chloride C4H4Cl2O2[3, 64]



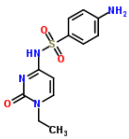
Compound Data

Melting point	**18.50 °C**	**291.65 K**			
CSID	13867055	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	154.9794	**H bond donors**	0	**ACD/LogP**	1.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	1.39 g/cm^3
SMILES	ClC(=O)CCC(Cl)=O				
STD InChIKey	IRXBNHGNHKNOJI-UHFFFAOYAK				

Melting Points

mp °C	source
17.00	Alfa Aesar
20.00	PHYSPROP

sulfacytine C12H14N4O3S[32, 64]



Compound Data

Melting point	**166.88 °C**	**440.02 K**			
CSID	5131	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	294.3296	**H bond donors**	3	**ACD/LogP**	-0.49
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.45 g/cm^3
SMILES	O=C1/N=C(\C=C/N1CC)NS(=O)(=O)c2ccc(N)cc2				
STD InChIKey	SIBQAECNSSQUOD-UHFFFAOYAA				

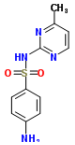
Melting Points

mp °C	source
166.50	DrugBank

167.25	PHYSPROP

sulfamerazine C11H12N4O2S[3, 9, 32, 44, 63, 63, 64]

Compound Data



Melting point	**235.58 °C**	**508.73 K**			
CSID	5134	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	264.3036	**H bond donors**	3	**ACD/LogP**	0.34
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.44 g/cm^3
SMILES	O=S(=O)(Nc1nc(ccn1)C)c2ccc(N)cc2				
STD InChIKey	QPPBRPIAZZHUNT-UHFFFAOYAN				

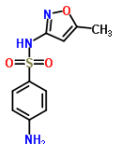
Melting Points

mp °C	source
236.00	Alfa Aesar
234.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
236.00	DrugBank
236.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
235.00	Patent 7766979
236.00	PHYSPROP
	Values not used in calculating the average melting point
170.00	Patent 7766979[1]

1. possibly for uncommon polymorph

sulfamethoxazole C10H11N3O3S[32, 35, 44, 64]

Compound Data



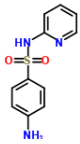
Melting point	**168.12 °C**	**441.27 K**			
CSID	5138	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	253.2776	**H bond donors**	3	**ACD/LogP**	0.89
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.46 g/cm^3
SMILES	O=S(=O)(Nc1noc(c1)C)c2ccc(N)cc2				
STD InChIKey	JLKIGFTWXXRPMT-UHFFFAOYAI				

Melting Points

mp °C	source
167.00	DrugBank
167.00	EPISuite-ChemSpider
171.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
167.00	PHYSPROP

sulfapyridine C11H11N3O2S[32, 61, 64]

Compound Data



Melting point	**191.83 °C**	**464.98 K**			
CSID	5145	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	249.2889	**H bond donors**	3	**ACD/LogP**	0.03
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.43 g/cm^3
SMILES	O=S(=O)(Nc1ncccc1)c2ccc(N)cc2				
STD InChIKey	GECHUMIMRBOMGK-UHFFFAOYAO				

Melting Points

mp °C	source
192.00	DrugBank
191.50	Oxford University MSDS
192.00	PHYSPROP

sulfolane C4H8O2S[3, 64]

Compound Data

Melting point	**27.30 °C**	**300.45 K**			
CSID	29080	**H bond acceptors**	2	**Rule of 5 violations**	0

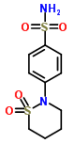
Molecular weight	120.1701	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.26 g/cm^3
SMILES	C1CCS(=O)(=O)C1				
STD InChIKey	HXJUTPCZVOIRIF-UHFFFAOYAA				

Melting Points

mp °C	source
27.00	Alfa Aesar
27.60	PHYSPROP

sulthiame C10H14N2O4S2[9, 64]

Compound Data



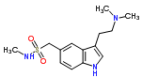
Melting point	**180.50 °C**	**453.65 K**			
CSID	5163	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	290.3592	**H bond donors**	2	**ACD/LogP**	-0.43
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	O=S2(=O)N(c1ccc(cc1)S(=O)(=O)N)CCCC2				
STD InChIKey	HMHVCUVYZFYAJI-UHFFFAOYAA				

Melting Points

mp °C	source
180.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
181.00	PHYSPROP

sumatriptan C14H21N3O2S[9, 32, 64]

Compound Data



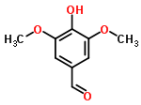
Melting point	**169.67 °C**	**442.82 K**			
CSID	5165	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	295.4004	**H bond donors**	2	**ACD/LogP**	0.67
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.24 g/cm^3
SMILES	O=S(=O)(NC)Cc1cc2c(cc1)ncc2CCN(C)C				
STD InChIKey	KQKPFRSPSRPDEB-UHFFFAOYAF				

Melting Points

mp °C	source
169.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
170.00	DrugBank
170.00	PHYSPROP

syringaldehyde C9H10O4[3, 64]

Compound Data



Melting point	**112.50 °C**	**385.65 K**			
CSID	8333	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.1733	**H bond donors**	1	**ACD/LogP**	1.30
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.24 g/cm^3
SMILES	COc1cc(cc(c1O)OC)C=O				
STD InChIKey	KCDXJAYRVLXPFO-UHFFFAOYAW				

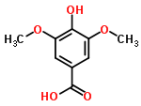
Melting Points

mp °C	source
112.00	Alfa Aesar
113.00	PHYSPROP

syringic acid C9H10O5[3, 61, 64]

Compound Data

Melting point	**206.50 °C**	**479.65 K**



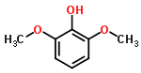
CSID	10289	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	198.1727	**H bond donors**	2	**ACD/LogP**	1.13
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.33 g/cm^3
SMILES	O=C(O)c1cc(OC)c(O)c(OC)c1				
STD InChIKey	JMSVCTWVEWCHDZ-UHFFFAOYAU				

Melting Points

mp °C	source
207.00	Alfa Aesar
205.00	Oxford University MSDS
207.50	PHYSPROP

syringol C8H10O3[2, 3, 64]

Compound Data



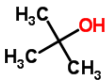
Melting point	**55.17 °C**	**328.32 K**			
CSID	6774	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	154.1632	**H bond donors**	1	**ACD/LogP**	0.77
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.13 g/cm^3
SMILES	O(c1cccc(OC)c1O)C				
STD InChIKey	KLIDCXVFHGNTTM-UHFFFAOYAG				

Melting Points

mp °C	source
55.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
54.00	Alfa Aesar
56.50	PHYSPROP

t-butanol C4H10O[3, 4, 61, 64]

Compound Data



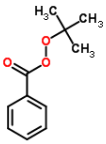
Melting point	**25.35 °C**	**298.50 K**			
CSID	6146	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	74.1216	**H bond donors**	1	**ACD/LogP**	0.58
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.81 g/cm^3
SMILES	CC(C)(C)O				
STD InChIKey	DKGAVHZHDRPRBM-UHFFFAOYAF				

Melting Points

mp °C	source
25.00	Alfa Aesar
26.00	American Petroleum Institute. Research Project 44; Selected ...
25.00	Oxford University MSDS
25.40	PHYSPROP

t-butyl benzenecarboperoxoate C11H14O3[3, 61, 64]

Compound Data

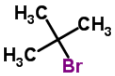


Melting point	**7.67 °C**	**280.82 K**			
CSID	11472	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	194.2271	**H bond donors**	0	**ACD/LogP**	3.33
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	1.06 g/cm^3
SMILES	O=C(OOC(C)(C)C)c1ccccc1				
STD InChIKey	GJBRNHKUVLOCEB-UHFFFAOYAT				

Melting Points

mp °C	source
7.00	Alfa Aesar
8.00	Oxford University MSDS
8.00	PHYSPROP

t-butyl bromide C4H9Br[3, 31, 64]



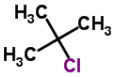
Compound Data

Melting point	**-17.40 °C**	**255.75 K**			
CSID	10053	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	137.0183	**H bond donors**	0	**ACD/LogP**	2.38
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.27 g/cm^3
SMILES	BrC(C)(C)C				
STD InChIKey	RKSOPLXZQNSWAS-UHFFFAOYAL				

Melting Points

mp °C	source
-20.00	Alfa Aesar
-16.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-16.20	PHYSPROP

t-butyl chloride C4H9Cl[3, 31, 61, 64]



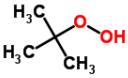
Compound Data

Melting point	**-25.75 °C**	**247.40 K**			
CSID	10054	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	92.5673	**H bond donors**	0	**ACD/LogP**	2.20
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3
SMILES	ClC(C)(C)C				
STD InChIKey	NBRKLOOSMBRFMH-UHFFFAOYAL				

Melting Points

mp °C	source
-26.00	Alfa Aesar
-25.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-26.00	Oxford University MSDS
-26.00	PHYSPROP

t-butyl hydroperoxide C4H10O2[61, 64]



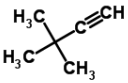
Compound Data

Melting point	**-5.50 °C**	**267.65 K**			
CSID	6170	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	90.121	**H bond donors**	1	**ACD/LogP**	1.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.92 g/cm^3
SMILES	CC(C)(C)OO				
STD InChIKey	CIHOLLKRGTVIJN-UHFFFAOYAX				

Melting Points

mp °C	source
-3.00	Oxford University MSDS
-8.00	PHYSPROP

t-butylacetylene C6H10[3, 4, 61, 64]



Compound Data

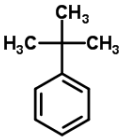
Melting point	**-78.05 °C**	**195.10 K**			
CSID	12924	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	82.1436	**H bond donors**	0	**ACD/LogP**	2.23
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.74 g/cm^3
SMILES	C#CC(C)(C)C				
STD InChIKey	PPWNCLVNXGCGAF-UHFFFAOYAJ				

Melting Points

mp °C	source
-78.00	Alfa Aesar
-78.00	American Petroleum Institute. Research Project 44; Selected ...
-78.00	Oxford University MSDS

-78.20	PHYSPROP

t-butylbenzene C10H14[3, 4, 61, 64]



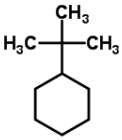
Compound Data

Melting point	**-58.33 °C**	**214.82 K**			
CSID	7088	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	134.2182	**H bond donors**	0	**ACD/LogP**	3.91
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.86 g/cm^3
SMILES	c1ccccc1C(C)(C)C				
STD InChIKey	YTZKOQUCBOVLHL-UHFFFAOYAK				

Melting Points

mp °C	source
-58.00	Alfa Aesar
-58.00	American Petroleum Institute. Research Project 44; Selected ...
-59.50	Oxford University MSDS
-57.80	PHYSPROP

t-butylcyclohexane C10H20[3, 64]



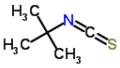
Compound Data

Melting point	**-41.10 °C**	**232.05 K**			
CSID	17481	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	140.2658	**H bond donors**	0	**ACD/LogP**	5.11
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.81 g/cm^3
SMILES	CC(C)(C)C1CCCCC1				
STD InChIKey	XTVMZZBLCLWBPM-UHFFFAOYAR				

Melting Points

mp °C	source
-41.00	Alfa Aesar
-41.20	PHYSPROP

t-butylisothiocyanate C5H9NS[3, 64]



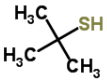
Compound Data

Melting point	**10.25 °C**	**283.40 K**			
CSID	11057	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	115.1967	**H bond donors**	0	**ACD/LogP**	2.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.89 g/cm^3
SMILES	S=C=N/C(C)(C)C				
STD InChIKey	ZFWFRTVIIMTOLY-UHFFFAOYAZ				

Melting Points

mp °C	source
10.00	Alfa Aesar
10.50	PHYSPROP

t-butylthiol C4H10S[4, 64]



Compound Data

Melting point	**0.25 °C**	**273.40 K**			
CSID	6147	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	90.1872	**H bond donors**	0	**ACD/LogP**	1.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	1	**Predicted density**	0.83 g/cm^3
SMILES	SC(C)(C)C				
STD InChIKey	WMXCDAVJEZZYLT-UHFFFAOYAT				

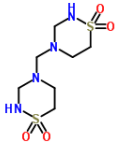
Melting Points

mp °C	source
1.00	American Petroleum Institute. Research Project 44; Selected ...

-0.50	PHYSPROP

taurolidine C7H16N4O4S2[9, 64]

Compound Data



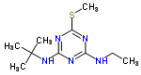
Melting point	**155.00 °C**	**428.15 K**			
CSID	27486	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	284.3563	**H bond donors**	2	**ACD/LogP**	-2.55
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.47 g/cm^3
SMILES	O=S2(=O)NCN(CN1CCS(=O)(=O)NC1)CC2				
STD InChIKey	AJKIRUJIDFJUKJ-UHFFFAOYAI				

Melting Points

mp °C	source
154.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
156.00	PHYSPROP

terbutrex C10H19N5S[61, 64, 70]

Compound Data



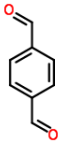
Melting point	**104.33 °C**	**377.48 K**			
CSID	12874	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	241.3564	**H bond donors**	2	**ACD/LogP**	3.44
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.13 g/cm^3
SMILES	S(c1nc(nc(n1)NC(C)(C)C)NCC)C				
STD InChIKey	IROINLKCQGIITA-UHFFFAOYAZ				

Melting Points

mp °C	source
104.00	Oxford University MSDS
104.00	PHYSPROP
105.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

terephthalaldehyde C8H6O2[2, 2, 3, 64]

Compound Data



Melting point	**116.00 °C**	**389.15 K**			
CSID	11673	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	134.132	**H bond donors**	0	**ACD/LogP**	1.49
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	O=Cc1ccc(C=O)cc1				
STD InChIKey	KUCOHFSKRZZVRO-UHFFFAOYAC				

Melting Points

mp °C	source
115.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
116.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
116.00	Alfa Aesar
117.00	PHYSPROP

terephthalonitrile C8H4N2[2, 3, 61, 64]

Compound Data

Melting point	**225.38 °C**	**498.52 K**			
CSID	11672	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.1308	**H bond donors**	0	**ACD/LogP**	1.51
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	c1cc(ccc1C#N)C#N				
STD InChIKey	BHXFKXOIODIUJO-UHFFFAOYAQ				

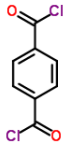
Melting Points

mp °C	source

226.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
226.00	Alfa Aesar
225.50	Oxford University MSDS
224.00	PHYSPROP

terephthaloyl chloride C8H4Cl2O2[3, 64]

Compound Data



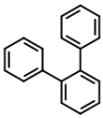
Melting point	**82.25 °C**	**355.40 K**			
CSID	7207	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	203.0222	**H bond donors**	0	**ACD/LogP**	2.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.43 g/cm^3
SMILES	O=C(Cl)c1ccc(C(Cl)=O)cc1				
STD InChIKey	LXEJRKJRKIFVNY-UHFFFAOYAY				

Melting Points

mp °C	source
81.00	Alfa Aesar
83.50	PHYSPROP

terphenyl C18H14[3, 7, 64]

Compound Data



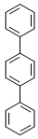
Melting point	**56.40 °C**	**329.55 K**			
CSID	6508	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	230.3038	**H bond donors**	0	**ACD/LogP**	5.27
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	c1cc(ccc1)c3ccccc3c2ccccc2				
STD InChIKey	OIAQMFOKAXHPNH-UHFFFAOYAT				

Melting Points

mp °C	source
57.00	Alfa Aesar
56.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
56.20	PHYSPROP

terphenyl C18H14[3, 7, 61, 64]

Compound Data



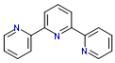
Melting point	**212.53 °C**	**485.67 K**			
CSID	6848	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	230.3038	**H bond donors**	0	**ACD/LogP**	5.63
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.05 g/cm^3
SMILES	c1cc(ccc1)c2ccc(cc2)c3ccccc3				
STD InChIKey	XJKSTNDFUHDPQJ-UHFFFAOYAJ				

Melting Points

mp °C	source
214.00	Alfa Aesar
213.00	Beilstein F. K.; Beilsteins Handbuch der Organischen Chemie....
213.00	Oxford University MSDS
210.10	PHYSPROP

terpyridine C15H11N3[3, 64]

Compound Data



Melting point	**90.50 °C**	**363.65 K**			
CSID	64012	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	233.2679	**H bond donors**	0	**ACD/LogP**	2.18
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.17 g/cm^3
SMILES	c1ccnc(c1)c2cccc(n2)c3ccccn3				

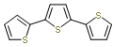
STD InChIKey	DRGAZIDRYFYHIJ-UHFFFAOYAP

Melting Points

mp °C	source
91.00	Alfa Aesar
90.00	PHYSPROP

terthienyl C12H8S3[3, 64]

Compound Data



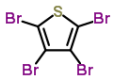
Melting point	**92.75 °C**	**365.90 K**			
CSID	58578	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	248.3869	**H bond donors**	0	**ACD/LogP**	5.56
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.32 g/cm^3
SMILES	s1cccc1c2sc(cc2)c3sccc3				
STD InChIKey	KXSFECAJUBPPFE-UHFFFAOYAI				

Melting Points

mp °C	source
92.00	Alfa Aesar
93.50	PHYSPROP

tetrabromothiophene C4Br4S[3, 64]

Compound Data



Melting point	**116.25 °C**	**389.40 K**			
CSID	69970	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	399.7238	**H bond donors**	0	**ACD/LogP**	4.51
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	2.78 g/cm^3
SMILES	Brc1sc(Br)c(Br)c1Br				
STD InChIKey	AVPWUAFYDNQGNZ-UHFFFAOYAI				

Melting Points

mp °C	source
115.00	Alfa Aesar
117.50	PHYSPROP

tetrachloroethylene C2Cl4[3, 64]

Compound Data

Melting point	**-22.15 °C**	**251.00 K**			
CSID	13837281	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	165.8334	**H bond donors**	0	**ACD/LogP**	2.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.65 g/cm^3
SMILES	Cl/C(Cl)=C(/Cl)Cl				
STD InChIKey	CYTYCFOTNPOANT-UHFFFAOYAO				

Melting Points

mp °C	source
-22.00	Alfa Aesar
-22.30	PHYSPROP

tetrachloromethane CCl4[31, 56, 58, 61, 61, 64, 69, 81]

Compound Data

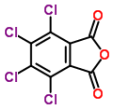
Melting point	**-22.99 °C**	**250.16 K**			
CSID	5730	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	153.8227	**H bond donors**	0	**ACD/LogP**	2.86
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.70 g/cm^3
SMILES	ClC(Cl)(Cl)Cl				
STD InChIKey	VZGDMQKNWNREIO-UHFFFAOYAV				

Melting Points

mp °C	source
-23.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-23.00	Merck Index
-23.00	NIOSH
-23.00	Oxford University MSDS
-23.00	Oxford University MSDS
-23.00	PHYSPROP
-23.00	Santa Cruz Biotechnology
-22.92	Wikipedia

tetrachlorophthalic anhydride C8Cl4O3[3, 61, 64]

Compound Data



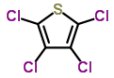
Melting point	**255.33 °C**	**528.48 K**			
CSID	8023	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	285.8958	**H bond donors**	0	**ACD/LogP**	3.56
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.90 g/cm^3
SMILES	O=C1OC(=O)c2c1c(Cl)c(Cl)c(Cl)c2Cl				
STD InChIKey	AUHHYELHRWCWEZ-UHFFFAOYAF				

Melting Points

mp °C	source
256.00	Alfa Aesar
255.50	Oxford University MSDS
254.50	PHYSPROP

tetrachlorothiophene C4Cl4S[3, 64]

Compound Data



Melting point	**29.25 °C**	**302.40 K**			
CSID	20971	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	221.9198	**H bond donors**	0	**ACD/LogP**	4.15
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.75 g/cm^3
SMILES	Clc1sc(Cl)c(Cl)c1Cl				
STD InChIKey	WZXXZHONLFRKGG-UHFFFAOYAU				

Melting Points

mp °C	source
28.00	Alfa Aesar
30.50	PHYSPROP

tetracontane C40H82[3, 64]

Compound Data

Melting point	**81.50 °C**	**354.65 K**			
CSID	18983	**H bond acceptors**	0	**Rule of 5 violations**	2
Molecular weight	563.0791	**H bond donors**	0	**ACD/LogP**	22.01
Phase 25 °C	solid	**Rotatable bonds**	37	**Predicted density**	0.82 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC				
STD InChIKey	KUPLEGDPSCCPJI-UHFFFAOYAV				

Melting Points

mp °C	source
81.00	Alfa Aesar
82.00	PHYSPROP

tetracosane C24H50[3, 64]

Compound Data

Melting point	**52.50 °C**	**325.65 K**			
CSID	12072	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	338.6538	**H bond donors**	0	**ACD/LogP**	13.51

Phase 25 °C	solid	**Rotatable bonds**	21	**Predicted density**	0.80 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCC)CCCC				
STD InChIKey	POOSGDOYLQNASK-UHFFFAOYAT				

Melting Points

mp °C	source
51.00	Alfa Aesar
54.00	PHYSPROP

tetracyanoethylene C6N4[3, 64]

Compound Data

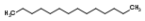
Melting point	**198.50 °C**	**471.65 K**			
CSID	12114	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	128.091	**H bond donors**	0	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.36 g/cm^3
SMILES	C(#N)C(=C(C#N)C#N)C#N				
STD InChIKey	NLDYACGHTUPAQU-UHFFFAOYAN				

Melting Points

mp °C	source
198.00	Alfa Aesar
199.00	PHYSPROP

tetradecane C14H30[3, 4, 61, 64]

Compound Data



Melting point	**5.83 °C**	**278.97 K**			
CSID	11883	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	198.388	**H bond donors**	0	**ACD/LogP**	8.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.76 g/cm^3
SMILES	C(CCCCC)CCCCCCCC				
STD InChIKey	BGHCVCJVXZWKCC-UHFFFAOYAQ				

Melting Points

mp °C	source
6.00	Alfa Aesar
6.00	American Petroleum Institute. Research Project 44; Selected ...
5.50	Oxford University MSDS
5.80	PHYSPROP

tetradecyl aldehyde C14H28O[2, 64]

Compound Data

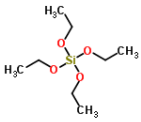
Melting point	**22.25 °C**	**295.40 K**			
CSID	29031	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	212.3715	**H bond donors**	0	**ACD/LogP**	6.01
Phase 25 °C	liquid/gas	**Rotatable bonds**	12	**Predicted density**	0.83 g/cm^3
SMILES	CCCCCCCCCCCCCC=O				
STD InChIKey	UHUFTBALEZWWIH-UHFFFAOYAK				

Melting Points

mp °C	source
24.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
20.50	PHYSPROP

tetraethyl orthosilicate C8H20O4Si[3, 61, 64]

Compound Data



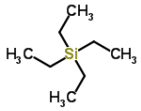
Melting point	**-84.50 °C**	**188.65 K**			
CSID	6270	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	208.3275	**H bond donors**	0	**ACD/LogP**	3.81
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.94 g/cm^3
SMILES	CCO[Si](OCC)(OCC)OCC				
STD InChIKey	BOTDANWDWHJENH-UHFFFAOYAS				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-86.00	Oxford University MSDS
-82.50	PHYSPROP

tetraethylsilane C8H20Si[3, 64]

Compound Data



Melting point	**-82.25 °C**	**190.90 K**			
CSID	11919	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	144.3299	**H bond donors**	0	**ACD/LogP**	4.96
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.73 g/cm^3
SMILES	CC[Si](CC)(CC)CC				
STD InChIKey	VCZQFJFZMMALHB-UHFFFAOYAY				

Melting Points

mp °C	source
-82.00	Alfa Aesar
-82.50	PHYSPROP

tetrafluoromethane CF4[61, 64]

Compound Data

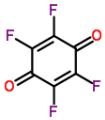
Melting point	**-183.80 °C**	**89.35 K**			
CSID	6153	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	88.0043	**H bond donors**	0	**ACD/LogP**	1.24
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.31 g/cm^3
SMILES	FC(F)(F)F				
STD InChIKey	TXEYQDLBPFQVAA-UHFFFAOYAJ				

Melting Points

mp °C	source
-184.00	Oxford University MSDS
-183.60	PHYSPROP

tetrafluoroquinone C6F4O2[61, 64]

Compound Data



Melting point	**181.50 °C**	**454.65 K**			
CSID	61540	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	180.0566	**H bond donors**	0	**ACD/LogP**	0.34
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.62 g/cm^3
SMILES	FC=1C(=O)C(\F)=C(\F)C(=O)C=1F				
STD InChIKey	JKLYZOGJWVAIQS-UHFFFAOYAA				

Melting Points

mp °C	source
179.00	Oxford University MSDS
184.00	PHYSPROP

tetrafluorosuccinic acid C4H2F4O4[3, 64]

Compound Data

Melting point	**117.00 °C**	**390.15 K**

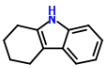
CSID	61150	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	190.0499	**H bond donors**	2	**ACD/LogP**	3.35
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.80 g/cm^3
SMILES	FC(F)(C(=O)O)C(F)(F)C(=O)O				
STD InChIKey	YUDUFRYTKFGQCL-UHFFFAOYAJ				

Melting Points

mp °C	source
115.00	Alfa Aesar
119.00	PHYSPROP

tetrahydrocarbazole C12H13N[3, 48, 64]

Compound Data



Melting point	**119.00 °C**	**392.15 K**			
CSID	13075	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	171.2383	**H bond donors**	1	**ACD/LogP**	3.83
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.15 g/cm^3
SMILES	c21c(cccc1)nc3c2CCCC3				
STD InChIKey	XKLNOVWDVMWTOB-UHFFFAOYAB				

Melting Points

mp °C	source
119.00	Alfa Aesar
118.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
120.00	PHYSPROP

tetrahydrofuran C4H8O[2, 3, 61, 64]

Compound Data

Melting point	**-108.11 °C**	**165.04 K**			
CSID	7737	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	72.1057	**H bond donors**	0	**ACD/LogP**	0.47
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.90 g/cm^3
SMILES	C1CCOC1				
STD InChIKey	WYURNTSHIVDZCO-UHFFFAOYAI				

Melting Points

mp °C	source
-108.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-108.00	Alfa Aesar
-108.00	Oxford University MSDS
-108.44	PHYSPROP

tetrahydropyran C5H10O[3, 32, 64]

Compound Data

Melting point	**-46.33 °C**	**226.82 K**			
CSID	8554	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	86.1323	**H bond donors**	0	**ACD/LogP**	0.89
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.88 g/cm^3
SMILES	O1CCCCC1				
STD InChIKey	DHXVGJBLRPWPCS-UHFFFAOYAV				

Melting Points

mp °C	source
-49.00	Alfa Aesar
-45.00	DrugBank
-45.00	PHYSPROP

tetrahydrothiophene C4H8S[3, 61, 64]

Compound Data

Melting point	**-96.03 °C**	**177.12 K**			
CSID	1095	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	88.1713	**H bond donors**	0	**ACD/LogP**	1.34
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.00 g/cm^3
SMILES	S1CCCC1				
STD InChIKey	RAOIDOHSFRTOEL-UHFFFAOYAY				

Melting Points

mp °C	source
-96.00	Alfa Aesar
-96.00	Oxford University MSDS
-96.10	PHYSPROP

tetralin C10H12[2, 3, 61, 64]

Compound Data

Melting point	**-34.42 °C**	**238.72 K**			
CSID	8097	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	132.2023	**H bond donors**	0	**ACD/LogP**	3.73
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.97 g/cm^3
SMILES	c1ccc2c(c1)CCCC2				
STD InChIKey	CXWXQJXEFPUFDZ-UHFFFAOYAG				

Melting Points

mp °C	source
-35.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
-36.00	Alfa Aesar
-31.00	Oxford University MSDS
-35.70	PHYSPROP

tetralone C10H10O[3, 64]

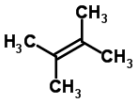
Compound Data

Melting point	**7.50 °C**	**280.65 K**			
CSID	10273	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	146.1858	**H bond donors**	0	**ACD/LogP**	2.61
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.10 g/cm^3
SMILES	O=C2c1c(cccc1)CCC2				
STD InChIKey	XHLHPRDBBAGVEG-UHFFFAOYAD				

Melting Points

mp °C	source
7.00	Alfa Aesar
8.00	PHYSPROP

tetramethylethylene C6H12[3, 4, 64]



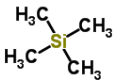
Compound Data

Melting point	**-74.53 °C**	**198.62 K**			
CSID	10776	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1595	**H bond donors**	0	**ACD/LogP**	3.17
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.70 g/cm^3
SMILES	CC(=C(C)C)C				
STD InChIKey	WGLLSSPDPJPLOR-UHFFFAOYAG				

Melting Points

mp °C	source
-75.00	Alfa Aesar
-74.00	American Petroleum Institute. Research Project 44; Selected ...
-74.60	PHYSPROP

tetramethylsilane C4H12Si[3, 64]



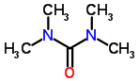
Compound Data

Melting point	**-99.50 °C**	**173.65 K**			
CSID	6156	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	88.2236	**H bond donors**	0	**ACD/LogP**	2.84
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.68 g/cm^3
SMILES	C[Si](C)(C)C				
STD InChIKey	CZDYPVPMEAXLPK-UHFFFAOYAT				

Melting Points

mp °C	source
-100.00	Alfa Aesar
-99.00	PHYSPROP

tetramethylurea C5H12N2O[3, 64]



Compound Data

Melting point	**-1.10 °C**	**272.05 K**			
CSID	11930	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	116.1616	**H bond donors**	0	**ACD/LogP**	0.19
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.95 g/cm^3
SMILES	O=C(N(C)C)N(C)C				
STD InChIKey	AVQQQNCBBIEMEU-UHFFFAOYAZ				

Melting Points

mp °C	source
-1.00	Alfa Aesar
-1.20	PHYSPROP

tetranitromethane CN4O8[61, 64]

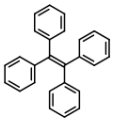
Compound Data

Melting point	**13.90 °C**	**287.05 K**			
CSID	13842838	**H bond acceptors**	12	**Rule of 5 violations**	2
Molecular weight	196.03	**H bond donors**	0	**ACD/LogP**	8.49
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	2.04 g/cm^3
SMILES	C([N+](=O)[O-])([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]				
STD InChIKey	NYTOUQBROMCLBJ-UHFFFAOYAA				

Melting Points

mp °C	source
14.00	Oxford University MSDS
13.80	PHYSPROP

tetraphenylethene C26H20[3, 64]



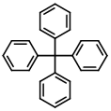
Compound Data

Melting point	**224.50 °C**	**497.65 K**			
CSID	62645	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	332.437	**H bond donors**	0	**ACD/LogP**	6.15
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.09 g/cm^3
SMILES	c1ccc(cc1)C(=C(c2ccccc2)c3ccccc3)c4ccccc4				
STD InChIKey	JLZUZNKTTIRERF-UHFFFAOYAF				

Melting Points

mp °C	source
224.00	Alfa Aesar
225.00	PHYSPROP

tetraphenylmethane C25H20[3, 64]



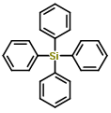
Compound Data

Melting point	**282.50 °C**	**555.65 K**			
CSID	11917	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	320.4263	**H bond donors**	0	**ACD/LogP**	7.31
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.08 g/cm^3
SMILES	c1c(cccc1)C(c2ccccc2)(c3ccccc3)c4ccccc4				
STD InChIKey	PEQHIRFAKIASBK-UHFFFAOYAS				

Melting Points

mp °C	source
283.00	Alfa Aesar
282.00	PHYSPROP

tetraphenylsilane C24H20Si[3, 64]



Compound Data

Melting point	**236.75 °C**	**509.90 K**			
CSID	59493	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	336.5011	**H bond donors**	0	**ACD/LogP**	8.18
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.10 g/cm^3
SMILES	c1c(cccc1)[Si](c2ccccc2)(c3ccccc3)c4ccccc4				
STD InChIKey	JLAVCPKULITDHO-UHFFFAOYAV				

Melting Points

mp °C	source
237.00	Alfa Aesar
236.50	PHYSPROP

tetratetracontane C44H90[3, 64]

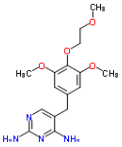
Compound Data

Melting point	**87.75 °C**	**360.90 K**			
CSID	21965	**H bond acceptors**	0	**Rule of 5 violations**	2
Molecular weight	619.1854	**H bond donors**	0	**ACD/LogP**	24.14
Phase 25 °C	solid	**Rotatable bonds**	41	**Predicted density**	0.82 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCCC				
STD InChIKey	KMXFZRSJMDYPPG-UHFFFAOYAJ				

Melting Points

mp °C	source
88.00	Alfa Aesar
87.50	PHYSPROP

tetroxoprim C16H22N4O4[44, 64]



Compound Data

Melting point	**154.25 °C**	**427.40 K**			
CSID	58910	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	334.3703	**H bond donors**	4	**ACD/LogP**	0.46
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.23 g/cm^3
SMILES	n1c(N)c(cnc1N)Cc2cc(OC)c(OCCOC)c(OC)c2				
STD InChIKey	WSWJIZXMAUYHOE-UHFFFAOYAT				

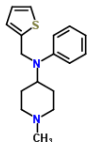
Melting Points

mp °C	source
154.50	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
154.00	PHYSPROP

thenaldine C17H22N2S[9, 64]

Compound Data

Melting point	**95.50 °C**	**368.65 K**



CSID	25957	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	286.435	**H bond donors**	0	**ACD/LogP**	4.28
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.14 g/cm^3
SMILES	s1c(ccc1)CN(c2ccccc2)C3CCN(C)CC3				
STD InChIKey	KLOHYVOVXOUKQI-UHFFFAOYAU				

Melting Points

mp °C	source
95.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
96.00	PHYSPROP

theophylline C7H8N4O2[9, 32, 44, 48, 61, 64, 70]

Compound Data

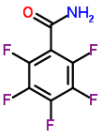
Melting point	**271.86 °C**	**545.01 K**			
CSID	2068	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	180.164	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.47 g/cm^3
SMILES	Cn1c2c(c(=O)n(c1=O)C)[nH]cn2				
STD InChIKey	ZFXYFBGIUFBOJW-UHFFFAOYAT				

Melting Points

mp °C	source
270.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
272.00	DrugBank
273.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
270.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
273.00	Oxford University MSDS
273.00	PHYSPROP
272.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

theophylline-7-acetic acid C7H2F5NO[3, 64]

Compound Data



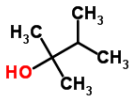
Melting point	**147.50 °C**	**420.65 K**			
CSID	62751	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	211.0889	**H bond donors**	2	**ACD/LogP**	0.97
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.63 g/cm^3
SMILES	Fc1c(c(F)c(F)c(F)c1F)C(=O)N				
STD InChIKey	WPWWHXPRJFDTTJ-UHFFFAOYAO				

Melting Points

mp °C	source
148.00	Alfa Aesar
147.00	PHYSPROP

thexyl alcohol C6H14O[4, 64]

Compound Data

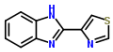


Melting point	**-12.00 °C**	**261.15 K**			
CSID	11180	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	102.1748	**H bond donors**	1	**ACD/LogP**	1.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.81 g/cm^3
SMILES	CC(C)C(C)(C)O				
STD InChIKey	IKECULIHBUCAKR-UHFFFAOYAD				

Melting Points

mp °C	source
-10.00	American Petroleum Institute. Research Project 44; Selected ...
-14.00	PHYSPROP

thiabendazole C10H7N3S[32, 61, 64]



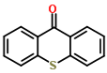
Compound Data

Melting point	**303.00 °C**	**576.15 K**			
CSID	5237	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	201.2477	**H bond donors**	1	**ACD/LogP**	2.47
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.41 g/cm^3
SMILES	n2c1c(cccc1)nc2c3ncsc3				
STD InChIKey	WJCNZQLZVWNLKY-UHFFFAOYAV				

Melting Points

mp °C	source
300.00	DrugBank
304.50	Oxford University MSDS
304.50	PHYSPROP

thiaxanthone C13H8OS[3, 48, 61, 64]



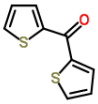
Compound Data

Melting point	**210.00 °C**	**483.15 K**			
CSID	9873	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	212.267	**H bond donors**	0	**ACD/LogP**	3.99
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.31 g/cm^3
SMILES	O=C1c3c(Sc2c1cccc2)cccc3				
STD InChIKey	YRHRIQCWCFGUEQ-UHFFFAOYAN				

Melting Points

mp °C	source
212.00	Alfa Aesar
210.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
209.00	Oxford University MSDS
209.00	PHYSPROP

thienone C9H6OS2[3, 64]



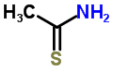
Compound Data

Melting point	**89.50 °C**	**362.65 K**			
CSID	62914	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	194.2733	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	O=C(c1sccc1)c2sccc2				
STD InChIKey	GUTQMBQKTSGBPQ-UHFFFAOYAO				

Melting Points

mp °C	source
89.00	Alfa Aesar
90.00	PHYSPROP

thioacetamide C2H5NS[3, 61, 64]



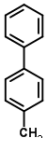
Compound Data

Melting point	**114.17 °C**	**387.32 K**			
CSID	2006126	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	75.1328	**H bond donors**	2	**ACD/LogP**	-0.26
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	S=C(N)C				
STD InChIKey	YUKQRDCYNOVPGJ-UHFFFAOYAD				

Melting Points

mp °C	source
112.00	Alfa Aesar
115.00	Oxford University MSDS
115.50	PHYSPROP

thioacetamide C13H12[3, 4, 64]



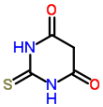
Compound Data

Melting point	**47.83 °C**	**320.98 K**			
CSID	12047	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	168.2344	**H bond donors**	0	**ACD/LogP**	4.63
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.98 g/cm^3
SMILES	Cc1ccc(cc1)c2ccccc2				
STD InChIKey	ZZLCFHIKESPLTH-UHFFFAOYAU				

Melting Points

mp °C	source
46.00	Alfa Aesar
48.00	American Petroleum Institute. Research Project 44; Selected ...
49.50	PHYSPROP

thiobarbituric acid C4H4N2O2S[61, 64]



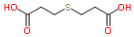
Compound Data

Melting point	**234.50 °C**	**507.65 K**			
CSID	2005830	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	144.1518	**H bond donors**	2	**ACD/LogP**	-0.52
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.57 g/cm^3
SMILES	O=C1NC(=S)NC(=O)C1				
STD InChIKey	RVBUGGBMJDPOST-UHFFFAOYAX				

Melting Points

mp °C	source
234.00	Oxford University MSDS
235.00	PHYSPROP

thiodipropionic acid C6H10O4S[3, 64]



Compound Data

Melting point	**130.00 °C**	**403.15 K**			
CSID	7805	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	178.2062	**H bond donors**	2	**ACD/LogP**	0.27
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.36 g/cm^3
SMILES	O=C(O)CCSCCC(=O)O				
STD InChIKey	ODJQKYXPKWQWNK-UHFFFAOYAG				

Melting Points

mp °C	source
131.00	Alfa Aesar
129.00	PHYSPROP

thiophene C4H4S[1, 3, 28, 36, 50, 61, 64, 72]

Compound Data

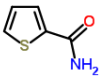
Melting point	**-38.28 °C**	**234.87 K**			
CSID	7739	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	84.1396	**H bond donors**	0	**ACD/LogP**	1.95
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.07 g/cm^3
SMILES	c1ccsc1				
STD InChIKey	YTPLMLYBLZKORZ-UHFFFAOYAY				

Melting Points

mp °C	source
-38.00	Acros
-38.00	Alfa Aesar
-38.21	CRC Handbook of Chemistry and Physics

-38.30	Fawcett FS; Rasmussen HE. Journal of the American Chemical S...
-38.30	Knovel
-38.00	Oxford University MSDS
-39.40	PHYSPROP
-38.00	Sigma-Aldrich

thiophene-2-carboxamide C5H5NOS[3, 64]



Compound Data

Melting point	**181.50 °C**	**454.65 K**			
CSID	20732	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	127.1643	**H bond donors**	2	**ACD/LogP**	0.52
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.30 g/cm^3
SMILES	O=C(N)c1sccc1				
STD InChIKey	DENPQNAWGQXKCU-UHFFFAOYAU				

Melting Points

mp °C	source
181.00	Alfa Aesar
182.00	PHYSPROP

thiophene-2-carboxylic acid C5H4O2S[3, 64]

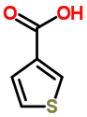
Compound Data

Melting point	**128.75 °C**	**401.90 K**			
CSID	10250	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.1491	**H bond donors**	1	**ACD/LogP**	1.57
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	O=C(O)c1sccc1				
STD InChIKey	QERYCTSHXKAMIS-UHFFFAOYAX				

Melting Points

mp °C	source
128.00	Alfa Aesar
129.50	PHYSPROP

thiophene-3-carboxylic acid C5H4O2S[3, 64]



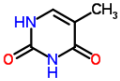
Compound Data

Melting point	**138.50 °C**	**411.65 K**			
CSID	6652	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	128.1491	**H bond donors**	1	**ACD/LogP**	1.48
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.40 g/cm^3
SMILES	c1cscc1C(=O)O				
STD InChIKey	YNVOMSDITJMNET-UHFFFAOYAE				

Melting Points

mp °C	source
139.00	Alfa Aesar
138.00	PHYSPROP

thymine C5H6N2O2[3, 44, 61, 64]



Compound Data

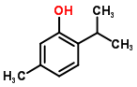
Melting point	**316.38 °C**	**589.52 K**			
CSID	1103	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	126.1133	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.23 g/cm^3
SMILES	Cc1c[nH]c(=O)[nH]c1=O				
STD InChIKey	RWQNBRDOKXIBIV-UHFFFAOYAL				

Melting Points

mp °C	source
317.00	Alfa Aesar
316.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
316.50	Oxford University MSDS
316.00	PHYSPROP

thymol C10H14O[3, 61, 64]

Compound Data



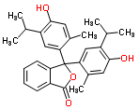
Melting point	**50.50 °C**	**323.65 K**			
CSID	21105998	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	150.2176	**H bond donors**	1	**ACD/LogP**	3.28
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.97 g/cm^3
SMILES	CC(C)c1ccc(C)cc1O				
STD InChIKey	MGSRCZKZVOBKFT-UHFFFAOYAS				

Melting Points

mp °C	source
51.00	Alfa Aesar
49.00	Oxford University MSDS
51.50	PHYSPROP

thymolphthalein C28H30O4[3, 61, 64]

Compound Data



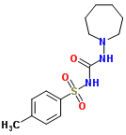
Melting point	**251.67 °C**	**524.82 K**			
CSID	29054	**H bond acceptors**	4	**Rule of 5 violations**	1
Molecular weight	430.5354	**H bond donors**	2	**ACD/LogP**	6.23
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.19 g/cm^3
SMILES	O=C1OC(c2ccccc12)(c3cc(c(O)cc3C)C(C)C)c4cc(c(O)cc4C)C(C)C				
STD InChIKey	LDKDGDIWEUUXSH-UHFFFAOYAV				

Melting Points

mp °C	source
252.00	Alfa Aesar
250.00	Oxford University MSDS
253.00	PHYSPROP

tolazamide C14H21N3O3S[9, 32, 64]

Compound Data



Melting point	**171.00 °C**	**444.15 K**			
CSID	5302	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	311.3998	**H bond donors**	2	**ACD/LogP**	1.71
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.29 g/cm^3
SMILES	O=S(=O)(c1ccc(cc1)C)NC(=O)NN2CCCCCC2				
STD InChIKey	OUDSBRTVNLOZBN-UHFFFAOYAL				

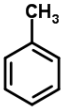
Melting Points

mp °C	source
170.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
171.50	DrugBank
171.50	PHYSPROP

toluene C7H8[3, 4, 61, 64]

Compound Data

Melting point	**-93.97 °C**	**179.17 K**			
CSID	1108	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	92.1384	**H bond donors**	0	**ACD/LogP**	2.72
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.87 g/cm^3



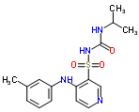
SMILES	Cc1ccccc1
STD InChIKey	YXFVVABEGXRONW-UHFFFAOYAT

Melting Points

mp °C	source
-93.00	Alfa Aesar
-95.00	American Petroleum Institute. Research Project 44; Selected ...
-93.00	Oxford University MSDS
-94.90	PHYSPROP

torsemide C16H20N4O3S[9, 32]

Compound Data



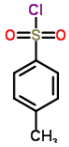
Melting point	**163.50 °C**	**436.65 K**			
CSID	38123	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	348.42	**H bond donors**	3	**ACD/LogP**	2.54
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.28 g/cm^3
SMILES	O=S(=O)(c2c(Nc1cc(ccc1)C)ccnc2)NC(=O)NC(C)C				
STD InChIKey	NGBFQHCMQULJNZ-UHFFFAOYAL				

Melting Points

mp °C	source
163.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
164.00	DrugBank

tosyl chloride C7H7ClO2S[2, 3, 61, 64]

Compound Data



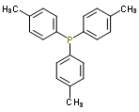
Melting point	**69.25 °C**	**342.40 K**			
CSID	7119	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	190.6473	**H bond donors**	0	**ACD/LogP**	2.45
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.34 g/cm^3
SMILES	O=S(Cl)(=O)c1ccc(cc1)C				
STD InChIKey	YYROPELSRYBVMQ-UHFFFAOYAN				

Melting Points

mp °C	source
69.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
69.00	Alfa Aesar
68.00	Oxford University MSDS
71.00	PHYSPROP

tri(4-tolyl)phosphine C21H21P[3, 64]

Compound Data



Melting point	**147.00 °C**	**420.15 K**			
CSID	13352	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	304.3652	**H bond donors**	0	**ACD/LogP**	7.07
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.00 g/cm^3
SMILES	c3c(P(c1ccc(cc1)C)c2ccc(cc2)C)ccc(c3)C				
STD InChIKey	WXAZIUYTQHYBFW-UHFFFAOYAP				

Melting Points

mp °C	source
145.00	Alfa Aesar
149.00	PHYSPROP

triacontane C30H62[3, 61, 64]

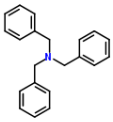
Compound Data

Melting point	**66.27 °C**	**339.42 K**			
CSID	12018	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	422.8133	**H bond donors**	0	**ACD/LogP**	16.70
Phase 25 °C	solid	**Rotatable bonds**	27	**Predicted density**	0.81 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCCCCC)CCCCCCC				
STD InChIKey	JXTPJDDICSTXJX-UHFFFAOYAO				

Melting Points

mp °C	source
67.00	Alfa Aesar
66.00	Oxford University MSDS
65.80	PHYSPROP

tribenzylamine C21H21N[3, 64]



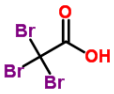
Compound Data

Melting point	**92.25 °C**	**365.40 K**			
CSID	22739	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	287.3981	**H bond donors**	0	**ACD/LogP**	5.67
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.07 g/cm^3
SMILES	N(Cc1ccccc1)(Cc2ccccc2)Cc3ccccc3				
STD InChIKey	MXHTZQSKTCCMFG-UHFFFAOYAF				

Melting Points

mp °C	source
93.00	Alfa Aesar
91.50	PHYSPROP

tribromoacetic acid C2HBr3O2[3, 61, 64]



Compound Data

Melting point	**131.83 °C**	**404.98 K**			
CSID	6175	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	296.7401	**H bond donors**	1	**ACD/LogP**	3.33
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	3.10 g/cm^3
SMILES	BrC(Br)(Br)C(=O)O				
STD InChIKey	QIONYIKHPASLHO-UHFFFAOYAS				

Melting Points

mp °C	source
132.00	Alfa Aesar
131.50	Oxford University MSDS
132.00	PHYSPROP

tribromofluoromethane CBr3F[3, 64]

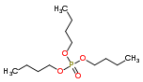
Compound Data

Melting point	**-73.80 °C**	**199.35 K**			
CSID	61026	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	270.7211	**H bond donors**	0	**ACD/LogP**	3.03
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	3.00 g/cm^3
SMILES	BrC(Br)(Br)F				
STD InChIKey	IHZAEIHJPNTART-UHFFFAOYAI				

Melting Points

mp °C	source
-74.00	Alfa Aesar
-73.60	PHYSPROP

tributyl phosphate C12H27O4P[3, 61, 64]



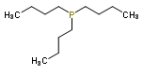
Compound Data

Melting point	**-79.67 °C**	**193.48 K**			
CSID	29090	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	266.3141	**H bond donors**	0	**ACD/LogP**	4.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	12	**Predicted density**	0.99 g/cm^3
SMILES	O=P(OCCCC)(OCCCC)OCCCC				
STD InChIKey	STCOOQWBFONSKY-UHFFFAOYAN				

Melting Points

mp °C	source
-80.00	Alfa Aesar
-80.00	Oxford University MSDS
-79.00	PHYSPROP

tributylphosphine C12H27P[3, 61]



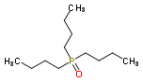
Compound Data

Melting point	**-62.50 °C**	**210.65 K**			
CSID	13231	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	202.3165	**H bond donors**	0	**ACD/LogP**	5.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.00 g/cm^3
SMILES	P(CCCC)(CCCC)CCCC				
STD InChIKey	TUQOTMZNTHZOKS-UHFFFAOYAQ				

Melting Points

mp °C	source
-65.00	Alfa Aesar
-60.00	Oxford University MSDS

tributylphosphine oxide C12H27OP[3, 64]



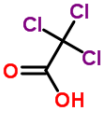
Compound Data

Melting point	**65.50 °C**	**338.65 K**			
CSID	12586	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	218.3159	**H bond donors**	0	**ACD/LogP**	4.14
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	0.87 g/cm^3
SMILES	CCCCP(=O)(CCCC)CCCC				
STD InChIKey	MNZAKDODWSQONA-UHFFFAOYAW				

Melting Points

mp °C	source
67.00	Alfa Aesar
64.00	PHYSPROP

trichloroacetic acid C2HCl3O2[3, 35, 61, 64]



Compound Data

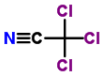
Melting point	**57.00 °C**	**330.15 K**			
CSID	10772050	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	163.3871	**H bond donors**	1	**ACD/LogP**	1.67
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.81 g/cm^3
SMILES	ClC(Cl)(Cl)C(O)=O				
STD InChIKey	YNJBWRMUSHSURL-UHFFFAOYAS				

Melting Points

mp °C	source
56.00	Alfa Aesar
57.50	EPISuite-ChemSpider
57.00	Oxford University MSDS
57.50	PHYSPROP

3, 61, 64

trichloroacetonitrile C2Cl3N



Compound Data

Melting point	**-42.67 °C**	**230.48 K**			
CSID	13861934	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	144.3871	**H bond donors**	0	**ACD/LogP**	2.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.62 g/cm^3
SMILES	ClC(Cl)(Cl)C#N				
STD InChIKey	DRUIESSIVFYOMK-UHFFFAOYAZ				

Melting Points

mp °C	source
-44.00	Alfa Aesar
-42.00	Oxford University MSDS
-42.00	PHYSPROP

trichloroacrylic acid C3HCl3O2[3, 64]

Compound Data

Melting point	**74.50 °C**	**347.65 K**			
CSID	10289059	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	175.3978	**H bond donors**	1	**ACD/LogP**	1.25
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.75 g/cm^3
SMILES	Cl/C(Cl)=C(/Cl)C(O)=O				
STD InChIKey	WMUBNWIGNSIRDH-UHFFFAOYAR				

Melting Points

mp °C	source
73.00	Alfa Aesar
76.00	PHYSPROP

trichlorofluoromethane CCl3F[61, 64]

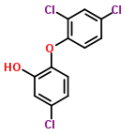
Compound Data

Melting point	**-110.80 °C**	**162.35 K**			
CSID	6149	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	137.3681	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.62 g/cm^3
SMILES	ClC(Cl)(Cl)F				
STD InChIKey	CYRMSUTZVYGINF-UHFFFAOYAT				

Melting Points

mp °C	source
-110.50	Oxford University MSDS
-111.10	PHYSPROP

triclosan C12H7Cl3O2[3, 61, 64]



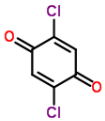
Compound Data

Melting point	**56.55 °C**	**329.70 K**			
CSID	5363	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	289.5418	**H bond donors**	1	**ACD/LogP**	5.17
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.49 g/cm^3
SMILES	Clc2cc(Cl)ccc2Oc1ccc(Cl)cc1O				
STD InChIKey	XEFQLINVKFYRCS-UHFFFAOYAS				

Melting Points

mp °C	source
57.00	Alfa Aesar
57.00	Oxford University MSDS
55.65	PHYSPROP

triclosan C6H2Cl2O2[3, 61]



Compound Data

Melting point	**160.75 °C**	**433.90 K**			
CSID	11516	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	176.9849	**H bond donors**	0	**ACD/LogP**	0.65
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.56 g/cm^3
SMILES	O=C\1C(\Cl)=C/C(=O)C(/Cl)=C/1				
STD InChIKey	LNXVNZRYYHFMEY-UHFFFAOYAG				

Melting Points

mp °C	source
160.00	Alfa Aesar
161.50	Oxford University MSDS

tricosane C23H48[3, 61, 64]

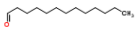
Compound Data

Melting point	**48.53 °C**	**321.68 K**			
CSID	12017	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	324.6272	**H bond donors**	0	**ACD/LogP**	12.98
Phase 25 °C	solid	**Rotatable bonds**	20	**Predicted density**	0.80 g/cm^3
SMILES	C(CCCCCCCCCCCCCCCCCCCC)CCC				
STD InChIKey	FIGVVZUWCLSUEI-UHFFFAOYAW				

Melting Points

mp °C	source
49.00	Alfa Aesar
49.00	Oxford University MSDS
47.60	PHYSPROP

tridecanal C13H26O[4, 64]



Compound Data

Melting point	**14.50 °C**	**287.65 K**			
CSID	23643	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	198.3449	**H bond donors**	0	**ACD/LogP**	5.69
Phase 25 °C	liquid/gas	**Rotatable bonds**	11	**Predicted density**	0.82 g/cm^3
SMILES	O=CCCCCCCCCCCCC				
STD InChIKey	BGEHHAVMRVXCGR-UHFFFAOYAF				

Melting Points

mp °C	source
15.00	American Petroleum Institute. Research Project 44; Selected ...
14.00	PHYSPROP

tridecane C13H28[3, 4, 61, 64]

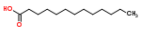
Compound Data

Melting point	**-5.08 °C**	**268.07 K**			
CSID	11882	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	184.3614	**H bond donors**	0	**ACD/LogP**	7.66
Phase 25 °C	liquid/gas	**Rotatable bonds**	10	**Predicted density**	0.76 g/cm^3
SMILES	C(CCCCCCCC)CCCC				
STD InChIKey	IIYFAKIEWZDVMP-UHFFFAOYAO				

Melting Points

mp °C	source
-5.00	Alfa Aesar
-5.00	American Petroleum Institute. Research Project 44; Selected ...
-5.00	Oxford University MSDS
-5.30	PHYSPROP

tridecanoic acid C13H26O2[32, 61, 64]



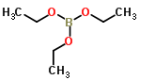
Compound Data

Melting point	**43.50 °C**	**316.65 K**			
CSID	12013	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	214.3443	**H bond donors**	1	**ACD/LogP**	5.56
Phase 25 °C	solid	**Rotatable bonds**	11	**Predicted density**	0.90 g/cm^3
SMILES	O=C(O)CCCCCCCCCCCC				
STD InChIKey	SZHOJFHSIKHZHA-UHFFFAOYAT				

Melting Points

mp °C	source
44.50	DrugBank
41.50	Oxford University MSDS
44.50	PHYSPROP

triethyl borate C6H15BO3[3, 64]



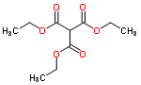
Compound Data

Melting point	**-84.90 °C**	**188.25 K**			
CSID	8659	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	145.9925	**H bond donors**	0	**ACD/LogP**	3.04
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.86 g/cm^3
SMILES	O(B(OCC)OCC)CC				
STD InChIKey	AJSTXXYNEIHPMD-UHFFFAOYAB				

Melting Points

mp °C	source
-85.00	Alfa Aesar
-84.80	PHYSPROP

triethyl methanetricarboxylate C10H16O6[3, 64]



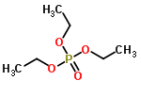
Compound Data

Melting point	**28.50 °C**	**301.65 K**			
CSID	72680	**H bond acceptors**	6	**Rule of 5 violations**	0
Molecular weight	232.2304	**H bond donors**	0	**ACD/LogP**	1.09
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	1.14 g/cm^3
SMILES	O=C(OCC)C(C(=O)OCC)C(=O)OCC				
STD InChIKey	AGZPNUZBDCYTBB-UHFFFAOYAQ				

Melting Points

mp °C	source
28.00	Alfa Aesar
29.00	PHYSPROP

triethyl phosphate C6H15O4P[61, 64]



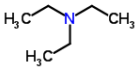
Compound Data

Melting point	**-56.20 °C**	**216.95 K**			
CSID	6287	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.1547	**H bond donors**	0	**ACD/LogP**	1.08
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	1.07 g/cm^3
SMILES	O=P(OCC)(OCC)OCC				
STD InChIKey	DQWPFSLDHJDLRL-UHFFFAOYAA				

Melting Points

mp °C	source
-56.00	Oxford University MSDS
-56.40	PHYSPROP

triethylamine C6H15N[3, 3, 28, 31, 45, 61, 64, 81, 84]



Compound Data

Melting point	**-114.90 °C**	**158.25 K**			
CSID	8158	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	101.19	**H bond donors**	0	**ACD/LogP**	1.65
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.75 g/cm^3
SMILES	CCN(CC)CC				
STD InChIKey	ZMANZCXQSJIPKH-UHFFFAOYAU				

Melting Points

mp °C	source
-115.00	Alfa Aesar
-115.00	Alfa Aesar
-114.70	CRC Handbook of Chemistry and Physics
-115.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-115.00	INCHEM
-115.00	Oxford University MSDS
-114.70	PHYSPROP
-114.70	Wikipedia
-115.00	Wolfram Alpha

triethylene glycol C6H14O4[3, 61, 64]

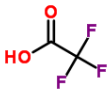
Compound Data

Melting point	**-6.00 °C**	**267.15 K**			
CSID	13835895	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	150.173	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	1.11 g/cm^3
SMILES	OCCOCCOCCO				
STD InChIKey	ZIBGPFATKBEMQZ-UHFFFAOYAS				

Melting Points

mp °C	source
-7.00	Alfa Aesar
-4.00	Oxford University MSDS
-7.00	PHYSPROP

trifluoroacetic acid C2HF3O2[3, 61, 64]



Compound Data

Melting point	**-15.07 °C**	**258.08 K**			
CSID	10239201	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	114.0233	**H bond donors**	1	**ACD/LogP**	1.35
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.57 g/cm^3
SMILES	C(=O)(C(F)(F)F)O				
STD InChIKey	DTQVDTLACAAQTR-UHFFFAOYAP				

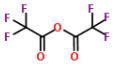
Melting Points

mp °C	source
-15.00	Alfa Aesar
-15.00	Oxford University MSDS
-15.20	PHYSPROP

trifluoroacetic anhydride C4F6O3[3, 61, 64]

Compound Data

Melting point	**-64.33 °C**	**208.82 K**			
CSID	21106178	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	210.0314	**H bond donors**	0	**ACD/LogP**	2.56
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.64 g/cm^3
SMILES	FC(F)(F)C(=O)OC(=O)C(F)(F)F				



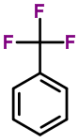
STD InChIKey	QAEDZJGFFMLHHQ-UHFFFAOYAX

Melting Points

mp °C	source
-65.00	Alfa Aesar
-63.00	Oxford University MSDS
-65.00	PHYSPROP

trifluoromethylbenzene C7H5F3[3, 61, 64]

Compound Data



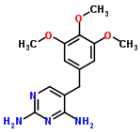
Melting point	**-28.37 °C**	**244.78 K**			
CSID	7090	**H bond acceptors**	0	**Rule of 5 violations**	0
Molecular weight	146.1098	**H bond donors**	0	**ACD/LogP**	2.89
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1ccc(cc1)C(F)(F)F				
STD InChIKey	GETTZEONDQJALK-UHFFFAOYAQ				

Melting Points

mp °C	source
-29.00	Alfa Aesar
-27.00	Oxford University MSDS
-29.10	PHYSPROP

trimethoprim C14H18N4O3[32, 35, 44, 61, 64]

Compound Data



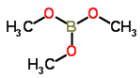
Melting point	**200.88 °C**	**474.03 K**			
CSID	5376	**H bond acceptors**	7	**Rule of 5 violations**	0
Molecular weight	290.3177	**H bond donors**	4	**ACD/LogP**	0.59
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.25 g/cm^3
SMILES	COc1cc(cc(c1OC)OC)Cc2cnc(nc2N)N				
STD InChIKey	IEDVJHCEMCRBQM-UHFFFAOYAV				

Melting Points

mp °C	source
201.00	DrugBank
201.00	EPISuite-ChemSpider
200.40	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
201.00	Oxford University MSDS
201.00	PHYSPROP

trimethyl borate C3H9BO3[3, 61, 64, 64]

Compound Data



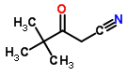
Melting point	**-32.82 °C**	**240.32 K**			
CSID	8157	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	103.9128	**H bond donors**	0	**ACD/LogP**	1.45
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.87 g/cm^3
SMILES	O(B(OC)OC)C				
STD InChIKey	WRECIMRULFAWHA-UHFFFAOYAY				

Melting Points

mp °C	source
-34.00	Alfa Aesar
-34.00	Oxford University MSDS
-29.30	PHYSPROP

-34.00	PHYSPROP

trimethylacetylacetonitrile C7H11NO[3, 64]



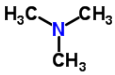
Compound Data

Melting point	**69.50 °C**	**342.65 K**			
CSID	97904	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	125.1683	**H bond donors**	0	**ACD/LogP**	0.55
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	0.93 g/cm^3
SMILES	N#CCC(=O)C(C)(C)C				
STD InChIKey	MXZMACXOMZKYHJ-UHFFFAOYAF				

Melting Points

mp °C	source
68.00	Alfa Aesar
71.00	PHYSPROP

trimethylamine C3H9N[61, 64]



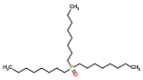
Compound Data

Melting point	**-117.04 °C**	**156.11 K**			
CSID	1114	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	59.1103	**H bond donors**	0	**ACD/LogP**	0.06
Phase 25 °C	liquid/gas	**Rotatable bonds**	0	**Predicted density**	0.69 g/cm^3
SMILES	N(C)(C)C				
STD InChIKey	GETQZCLCWQTVFV-UHFFFAOYAA				

Melting Points

mp °C	source
-117.00	Oxford University MSDS
-117.08	PHYSPROP

trioctylphosphine oxide C24H51OP[3, 61]



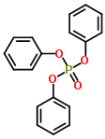
Compound Data

Melting point	**53.50 °C**	**326.65 K**			
CSID	59020	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	386.6349	**H bond donors**	0	**ACD/LogP**	10.25
Phase 25 °C	solid	**Rotatable bonds**	21	**Predicted density**	0.86 g/cm^3
SMILES	CCCCCCCCP(=O)(CCCCCCCC)CCCCCCCC				
STD InChIKey	ZMBHCYHQLYEYDV-UHFFFAOYAY				

Melting Points

mp °C	source
55.00	Alfa Aesar
52.00	Oxford University MSDS

triphenyl phosphate C18H15O4P[3, 61, 64]



Compound Data

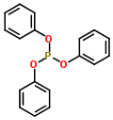
Melting point	**50.33 °C**	**323.48 K**			
CSID	7988	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	326.2831	**H bond donors**	0	**ACD/LogP**	4.10
Phase 25 °C	solid	**Rotatable bonds**	6	**Predicted density**	1.26 g/cm^3
SMILES	O=P(Oc1ccccc1)(Oc2ccccc2)Oc3ccccc3				
STD InChIKey	XZZNDPSIHUTMOC-UHFFFAOYAB				

Melting Points

mp °C	source
50.00	Alfa Aesar
50.50	Oxford University MSDS
50.50	PHYSPROP

triphenyl phosphite $C_{18}H_{15}O_3P$[3, 61, 64]

Compound Data



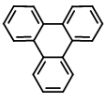
Melting point	**23.67 °C**	**296.82 K**			
CSID	7259	**H bond acceptors**	3	**Rule of 5 violations**	1
Molecular weight	310.2837	**H bond donors**	0	**ACD/LogP**	7.43
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.00 g/cm^3
SMILES	O(P(Oc1ccccc1)Oc2ccccc2)c3ccccc3				
STD InChIKey	HVLLSGMXQDNUAL-UHFFFAOYAF				

Melting Points

mp °C	source
23.00	Alfa Aesar
23.00	Oxford University MSDS
25.00	PHYSPROP

triphenylene $C_{18}H_{12}$[3, 44, 48, 64, 70]

Compound Data



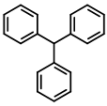
Melting point	**198.60 °C**	**471.75 K**			
CSID	8816	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	228.2879	**H bond donors**	0	**ACD/LogP**	5.73
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.19 g/cm^3
SMILES	c1ccc2c(c1)c3ccccc3c4c2cccc4				
STD InChIKey	SLGBZMMZGDRARJ-UHFFFAOYAN				

Melting Points

mp °C	source
197.00	Alfa Aesar
199.00	Hughes LD; Palmer DS; Nigsch F and Mitchell JBO. 2008 Why ar...
199.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
199.00	PHYSPROP
199.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

triphenylmethane $C_{19}H_{16}$[2, 3, 61, 64]

Compound Data



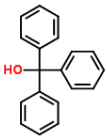
Melting point	**93.75 °C**	**366.90 K**			
CSID	10169	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	244.3303	**H bond donors**	0	**ACD/LogP**	5.69
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.05 g/cm^3
SMILES	c1c(cccc1)C(c2ccccc2)c3ccccc3				
STD InChIKey	AAAQKTZKLRYKHR-UHFFFAOYAF				

Melting Points

mp °C	source
94.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
93.00	Alfa Aesar
94.00	Oxford University MSDS
94.00	PHYSPROP

triphenylmethanol $C_{19}H_{16}O$[2, 3, 61, 64]

Compound Data

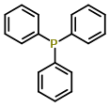


Melting point	**163.30 °C**	**436.45 K**			
CSID	6215	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	260.3297	**H bond donors**	1	**ACD/LogP**	4.59
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	OC(c1ccccc1)(c2ccccc2)c3ccccc3				
STD InChIKey	LZTRCELOJRDYMQ-UHFFFAOYAJ				

Melting Points

mp °C	source
163.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
163.00	Alfa Aesar
163.00	Oxford University MSDS
164.20	PHYSPROP

triphenylphosphine C18H15P[3, 61, 64]



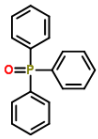
Compound Data

Melting point	**80.17 °C**	**353.32 K**			
CSID	11283	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	262.2855	**H bond donors**	0	**ACD/LogP**	5.69
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.00 g/cm^3
SMILES	c3c(P(c1ccccc1)c2ccccc2)cccc3				
STD InChIKey	RIOQSEWOXXDEQQ-UHFFFAOYAH				

Melting Points

mp °C	source
80.00	Alfa Aesar
80.50	Oxford University MSDS
80.00	PHYSPROP

triphenylphosphine oxide C18H15OP[3, 64]



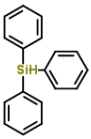
Compound Data

Melting point	**156.25 °C**	**429.40 K**			
CSID	12549	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	278.2849	**H bond donors**	0	**ACD/LogP**	2.87
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.17 g/cm^3
SMILES	O=P(c1ccccc1)(c2ccccc2)c3ccccc3				
STD InChIKey	FIQMHBFVRAXMOP-UHFFFAOYAB				

Melting Points

mp °C	source
156.00	Alfa Aesar
156.50	PHYSPROP

triphenylsilane C18H16Si[3, 64]



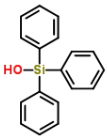
Compound Data

Melting point	**42.70 °C**	**315.85 K**			
CSID	63117	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	260.4051	**H bond donors**	0	**ACD/LogP**	7.01
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.00 g/cm^3
SMILES	c1c(cccc1)[SiH](c2ccccc2)c3ccccc3				
STD InChIKey	AKQNYQDSIDKVJZ-UHFFFAOYAL				

Melting Points

mp °C	source
43.00	Alfa Aesar
42.40	PHYSPROP

triphenylsilanol C18H16OSi[3, 64]



Compound Data

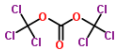
Melting point	**153.40 °C**	**426.55 K**			
CSID	63119	**H bond acceptors**	1	**Rule of 5 violations**	1
Molecular weight	276.4045	**H bond donors**	1	**ACD/LogP**	6.29
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.13 g/cm^3
SMILES	O[Si](c1ccccc1)(c2ccccc2)c3ccccc3				
STD InChIKey	NLSXASIDNWDYMI-UHFFFAOYAP				

Melting Points

mp °C	source
152.00	Alfa Aesar
154.80	PHYSPROP

triphosgene C3Cl6O3[3, 64]

Compound Data



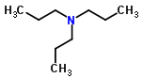
Melting point	**81.50 °C**	**354.65 K**			
CSID	85216	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	296.7483	**H bond donors**	0	**ACD/LogP**	4.02
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.90 g/cm^3
SMILES	ClC(Cl)(Cl)OC(=O)OC(Cl)(Cl)Cl				
STD InChIKey	UCPYLLCMEDAXFR-UHFFFAOYAA				

Melting Points

mp °C	source
84.00	Alfa Aesar
79.00	PHYSPROP

tripropylamine C9H21N[3, 31, 61, 64]

Compound Data



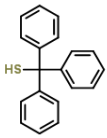
Melting point	**-93.50 °C**	**179.65 K**			
CSID	7334	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	143.2697	**H bond donors**	0	**ACD/LogP**	3.25
Phase 25 °C	liquid/gas	**Rotatable bonds**	6	**Predicted density**	0.78 g/cm^3
SMILES	N(CCC)(CCC)CCC				
STD InChIKey	YFTHZRPMJXBUME-UHFFFAOYAE				

Melting Points

mp °C	source
-93.00	Alfa Aesar
-94.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-93.50	Oxford University MSDS
-93.50	PHYSPROP

tritylthiol C19H16S[3, 64]

Compound Data



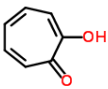
Melting point	**105.50 °C**	**378.65 K**			
CSID	69703	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	276.3953	**H bond donors**	0	**ACD/LogP**	6.83
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.12 g/cm^3
SMILES	SC(c1ccccc1)(c2ccccc2)c3ccccc3				
STD InChIKey	JQZIKLPHXXBMCA-UHFFFAOYAZ				

Melting Points

mp °C	source
106.00	Alfa Aesar
105.00	PHYSPROP

tropolone C7H6O2[3, 64]

Compound Data



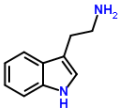
Melting point	**51.90 °C**	**325.05 K**			
CSID	10333	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	122.1213	**H bond donors**	1	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.28 g/cm^3
SMILES	c1ccc(c(=O)cc1)O				
STD InChIKey	MDYOLVRUBBJPFM-UHFFFAOYAW				

Melting Points

mp °C	source
53.00	Alfa Aesar
50.80	PHYSPROP

tryptamine C10H12N2[3, 64]

Compound Data



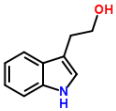
Melting point	**116.00 °C**	**389.15 K**			
CSID	1118	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	160.2157	**H bond donors**	3	**ACD/LogP**	1.54
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.16 g/cm^3
SMILES	c1ccc2c(c1)c(c[nH]2)CCN				
STD InChIKey	APJYDQYYACXCRM-UHFFFAOYAU				

Melting Points

mp °C	source
114.00	Alfa Aesar
118.00	PHYSPROP

tryptophol C10H11NO[3, 64]

Compound Data



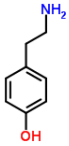
Melting point	**58.50 °C**	**331.65 K**			
CSID	10235	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	161.2004	**H bond donors**	2	**ACD/LogP**	1.64
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.22 g/cm^3
SMILES	c1ccc2c(c1)c(c[nH]2)CCO				
STD InChIKey	MBBOMCVGYCRMEA-UHFFFAOYAB				

Melting Points

mp °C	source
58.00	Alfa Aesar
59.00	PHYSPROP

tyramine C8H11NO[9, 48, 64]

Compound Data



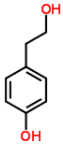
Melting point	**164.17 °C**	**437.32 K**			
CSID	5408	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	137.179	**H bond donors**	3	**ACD/LogP**	0.72
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.10 g/cm^3
SMILES	Oc1ccc(cc1)CCN				
STD InChIKey	DZGWFCGJZKJUFP-UHFFFAOYAB				

Melting Points

mp °C	source
164.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
164.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
164.50	PHYSPROP

tyrosol C8H10O2[3, 64]

Compound Data



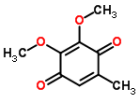
Melting point	**90.50 °C**	**363.65 K**			
CSID	9964	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	138.1638	**H bond donors**	2	**ACD/LogP**	0.62
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.17 g/cm^3
SMILES	Oc1ccc(cc1)CCO				
STD InChIKey	YCCILVSKPBXVIP-UHFFFAOYAG				

Melting Points

mp °C	source
91.00	Alfa Aesar
90.00	PHYSPROP

ubiquinone q0 C9H10O4[3, 61, 64]

Compound Data



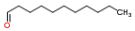
Melting point	**59.00 °C**	**332.15 K**			
CSID	62289	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	182.1733	**H bond donors**	0	**ACD/LogP**	0.12
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.19 g/cm^3
SMILES	O=C1/C=C(\C(=O)C(\OC)=C1\OC)C				
STD InChIKey	UIXPTCZPFCVOQF-UHFFFAOYAX				

Melting Points

mp °C	source
59.00	Alfa Aesar
58.50	Oxford University MSDS
59.50	PHYSPROP

undecanal C11H22O[3, 4, 64]

Compound Data



Melting point	**-2.00 °C**	**271.15 K**			
CSID	7894	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	170.2918	**H bond donors**	0	**ACD/LogP**	4.63
Phase 25 °C	liquid/gas	**Rotatable bonds**	9	**Predicted density**	0.82 g/cm^3
SMILES	O=CCCCCCCCCCC				
STD InChIKey	KMPQYAYAQWNLME-UHFFFAOYAE				

Melting Points

mp °C	source
-2.00	Alfa Aesar
0.00	American Petroleum Institute. Research Project 44; Selected ...
-4.00	PHYSPROP

undecane C11H24[3, 4, 61, 64]

Compound Data

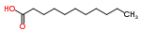
Melting point	**-25.90 °C**	**247.25 K**			
CSID	13619	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	156.3083	**H bond donors**	0	**ACD/LogP**	6.60
Phase 25 °C	liquid/gas	**Rotatable bonds**	8	**Predicted density**	0.74 g/cm^3
SMILES	C(CCCCCCCC)CC				
STD InChIKey	RSJKGSCJYJTIGS-UHFFFAOYAC				

Melting Points

mp °C	source
-26.00	Alfa Aesar
-26.00	American Petroleum Institute. Research Project 44; Selected ...
-26.00	Oxford University MSDS
-25.60	PHYSPROP

undecanoic acid C11H22O2[3, 35, 61, 64]

Compound Data



Melting point	**28.42 °C**	**301.57 K**			
CSID	7888	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	186.2912	**H bond donors**	1	**ACD/LogP**	4.50
Phase 25 °C	solid	**Rotatable bonds**	9	**Predicted density**	0.91 g/cm^3
SMILES	O=C(O)CCCCCCCCCC				

STD InChIKey	ZDPHROOEEOARMN-UHFFFAOYAS

Melting Points

mp °C	source
28.00	Alfa Aesar
28.60	EPISuite-ChemSpider
28.50	Oxford University MSDS
28.60	PHYSPROP

unizole C5H7N3O2[3, 64, 70]

Compound Data

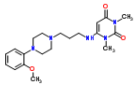
Melting point	**138.50 °C**	**411.65 K**			
CSID	2980	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	141.128	**H bond donors**	0	**ACD/LogP**	0.31
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.36 g/cm^3
SMILES	O=[N+]([O-])c1cnc(n1C)C				
STD InChIKey	IBXPYPUJPLLOIN-UHFFFAOYAK				

Melting Points

mp °C	source
137.00	Alfa Aesar
138.50	PHYSPROP
140.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

urapidil C20H29N5O3[9, 48, 64]

Compound Data



Melting point	**156.33 °C**	**429.48 K**			
CSID	5437	**H bond acceptors**	8	**Rule of 5 violations**	0
Molecular weight	387.476	**H bond donors**	1	**ACD/LogP**	2.28
Phase 25 °C	solid	**Rotatable bonds**	7	**Predicted density**	1.26 g/cm^3
SMILES	O=C1\C=C(/N(C(=O)N1C)C)NCCCN3CCN(c2ccccc2OC)CC3				
STD InChIKey	ICMGLRUYEQNHPF-UHFFFAOYAN				

Melting Points

mp °C	source
156.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
156.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
157.00	PHYSPROP

urea CH4N2O[3, 35, 61, 64]

Compound Data

Melting point	**133.85 °C**	**407.00 K**			
CSID	1143	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	60.0553	**H bond donors**	4	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.21 g/cm^3
SMILES	C(=O)(N)N				
STD InChIKey	XSQUKJJJFZCRTK-UHFFFAOYAF				

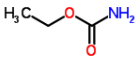
Melting Points

mp °C	source
134.00	Alfa Aesar
132.70	EPISuite-ChemSpider
136.00	Oxford University MSDS
132.70	PHYSPROP

urethane C3H7NO2[3, 32, 61, 64]

Compound Data

Melting point	**48.75 °C**	**321.90 K**



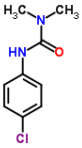
CSID	5439	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	89.0932	**H bond donors**	2	**ACD/LogP**	-0.15
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.04 g/cm^3
SMILES	O=C(OCC)N				
STD InChIKey	JOYRKODLDBILNP-UHFFFAOYAY				

Melting Points

mp °C	source
49.00	Alfa Aesar
49.00	DrugBank
48.00	Oxford University MSDS
49.00	PHYSPROP

urox C9H11ClN2O[3, 64, 70]

Compound Data



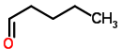
Melting point	**171.83 °C**	**444.98 K**			
CSID	8470	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	198.6494	**H bond donors**	1	**ACD/LogP**	1.89
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.25 g/cm^3
SMILES	Clc1ccc(NC(=O)N(C)C)cc1				
STD InChIKey	BMLIZLVNXIYGCK-UHFFFAOYAS				

Melting Points

mp °C	source
173.00	Alfa Aesar
170.50	PHYSPROP
172.00	Sepassi K; Yalkowsky SH. AAPS PharmSciTech 7(1) E1-E8 (2006)

valeraldehyde C5H10O[3, 4, 32, 61, 64]

Compound Data



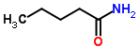
Melting point	**-91.50 °C**	**181.65 K**			
CSID	7772	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	86.1323	**H bond donors**	0	**ACD/LogP**	1.44
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.79 g/cm^3
SMILES	O=CCCCC				
STD InChIKey	HGBOYTHUEUWSSQ-UHFFFAOYAJ				

Melting Points

mp °C	source
-92.00	Alfa Aesar
-91.00	American Petroleum Institute. Research Project 44; Selected ...
-91.50	DrugBank
-91.50	Oxford University MSDS
-91.50	PHYSPROP

valeramide C5H11NO[3, 64]

Compound Data

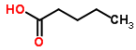


Melting point	**104.50 °C**	**377.65 K**			
CSID	11795	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	101.1469	**H bond donors**	2	**ACD/LogP**	0.36
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	0.90 g/cm^3
SMILES	O=C(N)CCCC				
STD InChIKey	IPWFJLQDVFKJDU-UHFFFAOYAM				

Melting Points

mp °C	source
103.00	Alfa Aesar
106.00	PHYSPROP

valeric acid C5H10O2[3, 4, 30, 32, 35, 54, 64]



Compound Data

Melting point	**-33.94 °C**	**239.21 K**			
CSID	7701	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	102.1317	**H bond donors**	1	**ACD/LogP**	1.31
Phase 25 °C	liquid/gas	**Rotatable bonds**	3	**Predicted density**	0.97 g/cm^3
SMILES	O=C(O)CCCC				
STD InChIKey	NQPDZGIKBAWPEJ-UHFFFAOYAU				

Melting Points

mp °C	source
-34.00	Alfa Aesar
-34.00	American Petroleum Institute. Research Project 44; Selected ...
-33.95	DellaGatta G; Jozwiak M; Ferloni P. Journal of Chemical Ther...
-34.00	DrugBank
-34.00	EPISuite-ChemSpider
-33.66	McDougall LA; Kilpatrick JE. Journal of Chemical Physics 42(...
-34.00	PHYSPROP

valeronitrile C5H9N[3, 31, 61, 64]

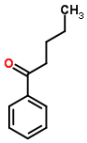
Compound Data

Melting point	**-96.05 °C**	**177.10 K**			
CSID	7770	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	83.1317	**H bond donors**	0	**ACD/LogP**	1.15
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	0.80 g/cm^3
SMILES	N#CCCCC				
STD InChIKey	RFFFKMOABOFIDF-UHFFFAOYAP				

Melting Points

mp °C	source
-96.00	Alfa Aesar
-96.00	Dreisbach R. R. Physical Properties of Chemical Compounds; V...
-96.00	Oxford University MSDS
-96.20	PHYSPROP

valerophenone C11H14O[3, 64]



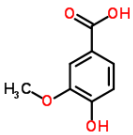
Compound Data

Melting point	**-9.20 °C**	**263.95 K**			
CSID	59482	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	162.2283	**H bond donors**	0	**ACD/LogP**	3.26
Phase 25 °C	liquid/gas	**Rotatable bonds**	4	**Predicted density**	0.95 g/cm^3
SMILES	O=C(c1ccccc1)CCCC				
STD InChIKey	XKGLSKVNOSHTAD-UHFFFAOYAK				

Melting Points

mp °C	source
-9.00	Alfa Aesar
-9.40	PHYSPROP

vanillic acid C8H8O4[3, 61, 64]



Compound Data

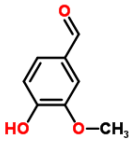
Melting point	**212.33 °C**	**485.48 K**			
CSID	8155	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	168.1467	**H bond donors**	2	**ACD/LogP**	1.30
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.35 g/cm^3
SMILES	COc1cc(ccc1O)C(=O)O				
STD InChIKey	WKOLLVMJNQIZCI-UHFFFAOYAH				

Melting Points

mp °C	source
214.00	Alfa Aesar
211.50	Oxford University MSDS
211.50	PHYSPROP

vanillin C8H8O3[3, 35, 61, 64]

Compound Data



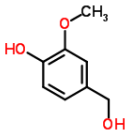
Melting point	**81.75 °C**	**354.90 K**			
CSID	13860434	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	152.1473	**H bond donors**	1	**ACD/LogP**	1.19
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.23 g/cm^3
SMILES	Oc1ccc(cc1OC)C=O				
STD InChIKey	MWOOGOJBHIARFG-UHFFFAOYAS				

Melting Points

mp °C	source
82.00	Alfa Aesar
81.50	EPISuite-ChemSpider
82.00	Oxford University MSDS
81.50	PHYSPROP

vanillyl alcohol C8H10O3[3, 61, 64]

Compound Data



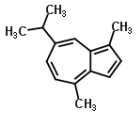
Melting point	**114.33 °C**	**387.48 K**			
CSID	56139	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	154.1632	**H bond donors**	2	**ACD/LogP**	0.00
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.23 g/cm^3
SMILES	Oc1ccc(cc1OC)CO				
STD InChIKey	ZENOXNGFMSCLLL-UHFFFAOYAV				

Melting Points

mp °C	source
114.00	Alfa Aesar
114.00	Oxford University MSDS
115.00	PHYSPROP

vaumigan C15H18[3, 64]

Compound Data



Melting point	**31.75 °C**	**304.90 K**			
CSID	3395	**H bond acceptors**	0	**Rule of 5 violations**	1
Molecular weight	198.3034	**H bond donors**	0	**ACD/LogP**	5.71
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	0.96 g/cm^3
SMILES	CC(C)c2cc1c(ccc1C)c(C)cc2				
STD InChIKey	FWKQNCXZGNBPFD-UHFFFAOYAG				

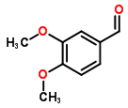
Melting Points

mp °C	source
32.00	Alfa Aesar
31.50	PHYSPROP

veratraldehyde C9H10O3[2, 3, 35, 64]

Compound Data

Melting point	**43.50 °C**	**316.65 K**			
CSID	21106008	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	166.1739	**H bond donors**	0	**ACD/LogP**	1.61
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.11 g/cm^3



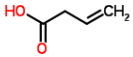
SMILES	COc1cc(ccc1OC)C=O
STD InChIKey	WJUFSDZVCOTFON-UHFFFAOYAT

Melting Points

mp °C	source
44.00	Aldrich Chemical Company; Aldrich Catalog-Handbook of Fine C...
44.00	Alfa Aesar
43.00	EPISuite-ChemSpider
43.00	PHYSPROP

vinylacetic acid C4H6O2[3, 64]

Compound Data



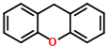
Melting point	**-37.00 °C**	**236.15 K**			
CSID	30349	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	86.0892	**H bond donors**	1	**ACD/LogP**	0.54
Phase 25 °C	liquid/gas	**Rotatable bonds**	2	**Predicted density**	1.02 g/cm^3
SMILES	O=C(O)C\C=C				
STD InChIKey	PVEOYINWKBTPIZ-UHFFFAOYAG				

Melting Points

mp °C	source
-39.00	Alfa Aesar
-35.00	PHYSPROP

xanthene C13H10O[28, 35, 61, 64, 72]

Compound Data



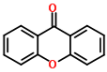
Melting point	**100.80 °C**	**373.95 K**			
CSID	6840	**H bond acceptors**	1	**Rule of 5 violations**	0
Molecular weight	182.2179	**H bond donors**	0	**ACD/LogP**	3.46
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.16 g/cm^3
SMILES	c1ccc2c(c1)Cc3ccccc3O2				
STD InChIKey	GJCOSYZMQJWQCA-UHFFFAOYAO				

Melting Points

mp °C	source
100.50	CRC Handbook of Chemistry and Physics
100.50	EPISuite-ChemSpider
101.00	Oxford University MSDS
100.50	PHYSPROP
101.50	Sigma-Aldrich

xanthone C13H8O2[3, 61]

Compound Data

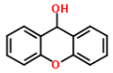


Melting point	**175.50 °C**	**448.65 K**			
CSID	6753	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	196.2014	**H bond donors**	0	**ACD/LogP**	3.39
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.28 g/cm^3
SMILES	O=C1c3c(Oc2c1cccc2)cccc3				
STD InChIKey	JNELGWHKGNBSMD-UHFFFAOYAA				

Melting Points

mp °C	source
176.00	Alfa Aesar
175.00	Oxford University MSDS

xanthydrol C13H10O2[3, 61, 64]



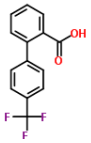
Compound Data

Melting point	**124.83 °C**	**397.98 K**			
CSID	65693	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	198.2173	**H bond donors**	1	**ACD/LogP**	2.27
Phase 25 °C	solid	**Rotatable bonds**	1	**Predicted density**	1.29 g/cm^3
SMILES	OC2c3c(Oc1c2cccc1)cccc3				
STD InChIKey	JFRMYMMIJXLMBB-UHFFFAOYAD				

Melting Points

mp °C	source
124.00	Alfa Aesar
123.00	Oxford University MSDS
127.50	PHYSPROP

xenalipin C14H9F3O2[3, 64]



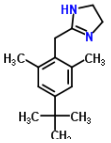
Compound Data

Melting point	**169.50 °C**	**442.65 K**			
CSID	49895	**H bond acceptors**	2	**Rule of 5 violations**	0
Molecular weight	266.2153	**H bond donors**	1	**ACD/LogP**	3.97
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.33 g/cm^3
SMILES	FC(F)(F)c1ccc(cc1)c2ccccc2C(=O)O				
STD InChIKey	IQOMYCGTGFGDFN-UHFFFAOYAA				

Melting Points

mp °C	source
169.00	Alfa Aesar
170.00	PHYSPROP

xylometazoline C16H24N2[9, 64]



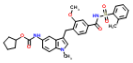
Compound Data

Melting point	**131.50 °C**	**404.65 K**			
CSID	5507	**H bond acceptors**	2	**Rule of 5 violations**	1
Molecular weight	244.3752	**H bond donors**	1	**ACD/LogP**	5.26
Phase 25 °C	solid	**Rotatable bonds**	3	**Predicted density**	1.00 g/cm^3
SMILES	N\1=C(\NCC/1)Cc2c(cc(cc2C)C(C)(C)C)C				
STD InChIKey	HUCJFAOMUPXHDK-UHFFFAOYAS				

Melting Points

mp °C	source
131.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
132.00	PHYSPROP

zafirlukast C31H33N3O6S[9, 32]



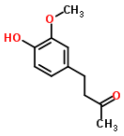
Compound Data

Melting point	**138.50 °C**	**411.65 K**			
CSID	5515	**H bond acceptors**	9	**Rule of 5 violations**	2
Molecular weight	575.6752	**H bond donors**	2	**ACD/LogP**	6.15
Phase 25 °C	solid	**Rotatable bonds**	8	**Predicted density**	1.32 g/cm^3
SMILES	O=S(=O)(c1ccccc1C)NC(=O)c2ccc(c(OC)c2)Cc4c3cc(ccc3n(c4)C)NC(=O)OC5CCCC5				
STD InChIKey	YEEZWCHGZNKEEK-UHFFFAOYAR				

Melting Points

mp °C	source
138.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
139.00	DrugBank

zingerone C11H14O3[3, 64]



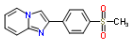
Compound Data

Melting point	**40.75 °C**	**313.90 K**			
CSID	28952	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	194.2271	**H bond donors**	1	**ACD/LogP**	0.64
Phase 25 °C	solid	**Rotatable bonds**	5	**Predicted density**	1.11 g/cm^3
SMILES	O=C(C)CCc1cc(OC)c(O)cc1				
STD InChIKey	OJYLAHXKWMRDGS-UHFFFAOYAN				

Melting Points

mp °C	source
41.00	Alfa Aesar
40.50	PHYSPROP

zolimidine C14H12N2O2S[9, 64]



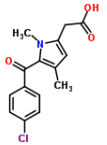
Compound Data

Melting point	**242.50 °C**	**515.65 K**			
CSID	13985	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	272.3223	**H bond donors**	0	**ACD/LogP**	2.13
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.31 g/cm^3
SMILES	O=S(=O)(c3ccc(c1nc2ccccn2c1)cc3)C				
STD InChIKey	VSLIUWLPFRVCDL-UHFFFAOYAK				

Melting Points

mp °C	source
242.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
243.00	PHYSPROP

zomepirac C15H14ClNO3[9, 32, 48, 64]



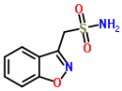
Compound Data

Melting point	**178.25 °C**	**451.40 K**			
CSID	5531	**H bond acceptors**	4	**Rule of 5 violations**	0
Molecular weight	291.7296	**H bond donors**	1	**ACD/LogP**	2.64
Phase 25 °C	solid	**Rotatable bonds**	4	**Predicted density**	1.28 g/cm^3
SMILES	O=C(c1c(cc(n1C)CC(=O)O)C)c2ccc(Cl)cc2				
STD InChIKey	ZXVNMYWKKDOREA-UHFFFAOYAX				

Melting Points

mp °C	source
178.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
178.50	DrugBank
178.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
178.50	PHYSPROP

zonisamide C8H8N2O3S[32, 64]



Compound Data

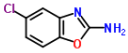
Melting point	**161.75 °C**	**434.90 K**			
CSID	5532	**H bond acceptors**	5	**Rule of 5 violations**	0
Molecular weight	212.2257	**H bond donors**	2	**ACD/LogP**	-0.10
Phase 25 °C	solid	**Rotatable bonds**	2	**Predicted density**	1.51 g/cm^3
SMILES	O=S(=O)(N)Cc2noc1ccccc12				
STD InChIKey	UBQNRHZMVUUOMG-UHFFFAOYAZ				

Melting Points

mp °C	source
162.00	DrugBank
161.50	PHYSPROP

zoxazolamine C7H5ClN2O[9, 48, 64]

Compound Data



Melting point	**184.17 °C**	**457.32 K**			
CSID	5878	**H bond acceptors**	3	**Rule of 5 violations**	0
Molecular weight	168.5804	**H bond donors**	2	**ACD/LogP**	2.46
Phase 25 °C	solid	**Rotatable bonds**	0	**Predicted density**	1.48 g/cm^3
SMILES	Clc1cc2nc(oc2cc1)N				
STD InChIKey	YGCODSQDUUUKIV-UHFFFAOYAA				

Melting Points

mp °C	source
184.00	Bergstrom C. A. S.; Norinder U.; Luthman K.; Artursson P. Mo...
184.00	Karthikeyan M.; Glen R.C.; Bender A. General melting point p...
184.50	PHYSPROP

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