Performance of the ALOGPS 2.1 program for octanol-water partition coefficient prediction with organic chemicals on the Canadian Domestic Substances List

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Octanol-water partition coefficients (K_{ow}) are widely used in environmental and biological chemistry to predict and understand the partitioning behavior of neutral organic compounds and their salts into a range of organic materials. Because of the time and expense in obtaining experimental K_{ow} data, a large number of freely available and commercial K_{ow} prediction software programs are available. One of the most popular K_{ow} prediction programs is KOWWIN, currently included as part of the EPI Suite environmental modeling program (<http://www.epa.gov/oppt/exposure/pubs/episuitd.html>). KOWWIN estimated K_{ow} values are used on the Domestic Substances List (DSL; http://www.ec.gc.ca/ceparegistry/Subs_list/Domestic.cfm) of Environment Canada for screening level assessments of bioaccumulation potential. In the current study, we examined the predictive capacity of KOWWIN against the ALOGPS 2.1 program (<http://www.vclab.org/lab/alogps/>; ref. [1-4]) – both freely available internet based programs – for substances on the Canadian DSL with and without comparative experimental K_{ow} values.

From an initial sample of 1771 experimental log K_{ow} values in the Canadian DSL listing, the removal of duplicate entries, errors, salts, and organosilicon compounds resulted in a reduced set of 1545 compounds (Appendix Table 1). The substantial number of errors and duplicates in the original source Canadian DSL experimental K_{ow} list necessitates rigorous pre-screening by researchers prior to use. The following three general categories of concern were encountered: (1) duplicate entries, often from different common names and IUPAC

naming formalisms that all refer to the same structure; (2) failure to properly specify geometrical isomerism (i.e., cis-/trans- and E-/Z- designation of various functional groups) or stereochemistry (i.e., R/S), both of which could have been designated using the SMILES notation [5, 6] in this database; and (3) while the compound name suggests the log K_{ow} value was determined/estimated for a salt, the SMILES formula indicates the molecular form, thereby making direct comparisons between experimental and estimated data invalid, and the use of the estimated data subject to significant uncertainty. For estimated K_{ow} values, neither KOWWIN nor ALOGPS distinguishes between E-/Z-isomer or diastereomer based differences in physicochemical properties.

The mean signed error (MSE), mean absolute error (MAE), and root mean squared error (RMSE) between experimental and estimated log K_{ow} values for KOWWIN on these 1545 compounds were 0.02, 0.26, and 0.37 units, respectively, compared to -0.02, 0.25, and 0.35 units, respectively for ALOGPS. By comparison, COSMOfrag was reported to have a RMSE of 0.74 log K_{ow} units using an unscreened version of the Canadian DSL. [7] KOWWIN and ALOGPS yield the following respective regression equations between predicted and experimental log K_{ow} values (Figure 1):

$$\log K_{ow,ALOGPS} = 0.961(\pm 0.004) \times \log K_{ow,expt} + 0.058(\pm 0.012) \dots (1)$$

$$n=1545, r=0.983, s=0.346, cv=0.182$$

$$\log K_{ow,KOWWIN} = 0.992(\pm 0.005) \times \log K_{ow,expt} + 0.033(\pm 0.013) \dots (2)$$

$$n=1545, r=0.982, s=0.368, cv=0.191$$

Log K_{ow} error residuals for KOWWIN are evenly distributed with no significant trend ($r=-0.04$, $p_{m=0}=0.12$, $p_{b=0}=0.01$). ALOGPS error residuals do display a significant trend ($r=-0.21$, $p_{m=0}<10^{-17}$, $p_{b=0}<10^{-5}$), generally decreasing in signed error magnitude with increasing log K_{ow} .

Compounds with log K_{ow} values >5 are often classified by regulatory agencies as having high bioaccumulation potential, provided they are sufficiently persistent in environmental and biological systems. Similarly, "Lipinski's Rule of Five" postulates that above a log K_{ow} of 5, poor absorption or permeation is anticipated in a drug discovery setting. [8] Of the 83 compounds on our screened version of the Canadian DSL with experimental log $K_{ow}>5$, KOWWIN correctly classified 75 and ALOGPS correctly classified 72. KOWWIN generated 11 false positives (i.e., predicting log $K_{ow}>5$ when experimental log $K_{ow}<5$) and 8 false negatives (i.e., predicting log $K_{ow}<5$ when experimental log $K_{ow}>5$). ALOGPS generated 8 false positives and 11 false negatives.

The Canadian DSL gives 9544 compounds without experimental log K_{ow} values, and for which KOWWIN estimates have been generated. A rudimentary screening of this list to remove duplicate entries, errors, salts, and organosilicon compounds resulted in a reduced set of 6529 compounds. A comparison of KOWWIN and ALOGPS estimated log K_{ow} values for these compounds indicates significant predictive differences between the two programs (Fig. 2), yielding a root mean squared deviation between the methods of 2.18 log K_{ow} units. Modest agreement exists between the programs at estimated log K_{ow} values from -5 to 5, but outside of this range the deviations between the two methods increase up to a maximum difference of 39.3 log K_{ow} units. Of particular interest, there are some compounds whose ALOGPS log K_{ow} estimates are <5, but the corresponding KOWWIN log K_{ow} estimates can range up to >28.

Fig. 1. Comparison between ALOGPS ((a)(i)) and KOWWIN ((b)(i)) predicted and experimental log K_{ow} values for compounds on the Canadian DSL and corresponding distributions of residual errors for the ALOGPS ((a)(ii)) and KOWWIN ((b)(ii)) estimates. 1:1 lines (dashed) are also given.

Fig. 2. Comparison between ALOGPS and KOWWIN estimated log K_{ow} values for compounds on the Canadian DSL without experimental K_{ow} data. A 1:1 line (dashed) is also given.

In some cases, ALOGPS estimates a log K_{ow} > 5, whereas KOWWIN gives a corresponding log K_{ow} estimate of less than -1. Consequently, the differences between the two programs are not restricted to log K_{ow} values that are clear environmental regulatory and/or drug discovery outliers (i.e., where both methods predict log K_{ow} > 10 or < 0), but also for a significant number of compounds where one method predicts a value well below a log K_{ow} of 5, and the other method predicts a value well above this cutoff, and vice versa.

References and Notes

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[1] Tetko, I.V.; Bruneau, P. "Application of ALOGPS to predict 1-octanol/water distribution coefficients, log P, and log D, of AstraZeneca in-house database." *J. Pharm. Sci.* **2004**, 93, 3103-3110.

[2] Tetko, I.V.; Poda, G.I. "Application of ALOGPS 2.1 to predict log D distribution coefficient for Pfizer proprietary compounds." *J. Med. Chem.* **2004**, 47, 5601-5604.

[3] Tetko, I.V. "Computing chemistry on the web." *Drug Discov. Today* **2005**, 10, 1497-1500.

[4] Tetko, I.V.; Gasteiger, J.; Todeschini, R.; Mauri, A.; Livingstone, D.; Ertl, P.; Palyulin, V.A.; Radchenko, E.V.; Zefirov, N.S.; Makarenko, A.S.; Tanchuk, V.Y.; Prokopenko, V.V. "Virtual computational chemistry laboratory: Design and description." *J. Comput. Aided Mol. Des.* **2005**, 19, 453-463.

[5] Weininger, D. "SMILES: A chemical language and information system. 1. Introduction to methodology and encoding rules." *J. Chem. Inf. Comp. Sci.* **1988**, 28, 31-36.

[6] Weininger, D.; Weininger, A.; Weininger, J.L. "SMILES. 2. Algorithm for generation of unique SMILES notation." *J. Chem. Inf. Comp. Sci.* **1989**, 29, 97-101.

[7] Wittekindt, C.; Goss, K.U. "Screening the partition behavior of a large number of chemicals with a quantum-chemical software." *Chemosphere* **2009**, 76, 460-464.

[8] Lipinski, C.A.; Lombardo, F.; Dominy, B.W.; Feeney, P.J. "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings." *Adv. Drug Deliv. Rev.* **2001**, 46, 3-26.

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Appendix Table 1. Comparison between experimentally obtained log K_{ow} values and corresponding KOWWIN and ALOGPS estimates and errors.

compound	SMILES	expt	KOWWIN		ALOGPS	
			estimate	error	estimate	error
cystine	<chem>O=C(O)C(N)CSSCC(N)C(=O)O</chem>	-5.08	-4.34	0.74	-3.16	1.92
ornithine	<chem>O=C(O)C(N)CCCN</chem>	-4.22	-3.48	0.74	-3.64	0.58
arginine	<chem>O=C(O)C(N)CCCNC(=N)N</chem>	-4.20	-4.00	0.20	-3.49	0.71
glycine, N-(phosphonomethyl)-	<chem>OC(=O)CNCPO(O)(O)=O</chem>	-4.00	-4.47	-0.47	-2.43	1.57
aspartic acid	<chem>O=C(O)C(N)CC(=O)O</chem>	-3.89	-4.32	-0.43	-3.52	0.37
asparagine	<chem>O=C(O)C(N)CC(=O)N</chem>	-3.82	-4.99	-1.17	-3.36	0.46
alpha-glucopyranoside,-fructofuranosyl	<chem>O(C(C(O)C(O)C1O)CO)C1OC(OC(C2O)CO)(C2O)CO</chem>	-3.70	-4.27	-0.57	-2.63	1.07
glutamic acid	<chem>O=C(O)C(N)CCC(=O)O</chem>	-3.69	-3.83	-0.14	-3.54	0.15
glutamine	<chem>O=C(O)C(N)CCC(=O)N</chem>	-3.64	-4.49	-0.85	-3.32	0.32
histidine	<chem>O=C(O)C(N)CC(N=CN1)=C1</chem>	-3.32	-3.22	0.10	-2.67	0.65
glucose	<chem>OCC1C(O)C(O)C(O)C(O)O1</chem>	-3.24	-2.89	0.35	-2.57	0.67
glycine	<chem>O=C(O)CN</chem>	-3.21	-3.41	-0.20	-3.34	-0.13
butanoic acid, 4-amino-	<chem>O=C(O)CCCN</chem>	-3.17	-3.60	-0.43	-2.99	0.18
proline, 4-hydroxy-	<chem>O=C(O)C(NCC1O)C1</chem>	-3.17	-2.69	0.48	-3.31	-0.14
mannitol	<chem>OCC(O)C(O)C(O)C(O)CO</chem>	-3.10	-3.01	0.09	-2.68	0.42
serine	<chem>O=C(O)C(N)CO</chem>	-3.07	-3.46	-0.39	-3.42	-0.35
alanine	<chem>O=C(O)CCN</chem>	-3.05	-4.09	-1.04	-3.26	-0.21
lysine	<chem>O=C(O)C(N)CCCCN</chem>	-3.05	-2.99	0.06	-3.76	-0.71
alanine	<chem>O=C(O)C(N)C</chem>	-2.96	-2.99	-0.03	-3.05	-0.09
hexanoic acid, 6-amino-	<chem>O=C(O)CCCCCN</chem>	-2.95	-2.62	0.33	-2.69	0.26
threonine	<chem>O=C(O)C(N)C(O)C</chem>	-2.94	-3.04	-0.10	-3.01	-0.07
glycine, N-glycyl-	<chem>O=C(NCC(=O)O)CN</chem>	-2.92	-2.09	0.83	-3.23	-0.31
glycine, N-methyl-	<chem>O=C(O)CNC</chem>	-2.78	-2.94	-0.16	-3.06	-0.28
hydrazinecarboxamide	<chem>NC(=O)NN</chem>	-2.75	-2.64	0.11	-1.88	0.87
proline	<chem>O=C(O)C(NCC1)C1</chem>	-2.54	-2.15	0.39	-2.71	-0.17
cytidine	<chem>O=C1N=C(N)C=CN1C2OC(CO)C(O)C2O</chem>	-2.51	-2.46	0.05	-2.18	0.33
cysteine	<chem>O=C(O)C(N)CS</chem>	-2.49	-3.05	-0.56	-2.57	-0.08
ribose	<chem>OCC1OC(O)C(O)C1O</chem>	-2.32	-2.43	-0.11	-2.65	-0.33
1,2,3,4-butanetetrol	<chem>OCC(O)C(O)CO</chem>	-2.29	-2.11	0.18	-2.03	0.26
valine	<chem>O=C(O)C(N)C(C)C</chem>	-2.26	-2.08	0.18	-2.29	-0.03
tyrosine	<chem>O=C(O)C(N)Cc(ccc(O)c1)c1</chem>	-2.26	-1.76	0.50	-2.39	-0.13
1H-purine-2,6,8(3H)-trione, 7,9-dihydro-	<chem>O=C1NC(=O)NC2=C1NC(=O)N2</chem>	-2.17	-1.46	0.71	-1.12	1.05
benzenesulfonic acid, 4-amino-	<chem>O=S(=O)(O)c(ccc(N)c1)c1</chem>	-2.16	-2.08	0.08	-1.35	0.81
norvaline	<chem>O=C(O)C(N)CCC</chem>	-2.11	-2.01	0.10	-2.04	0.07
urea	<chem>O=C(N)N</chem>	-2.11	-1.56	0.55	-1.78	0.33
1,2-ethanediamine	<chem>NCCN</chem>	-2.04	-1.62	0.42	-1.77	0.27
uridine	<chem>O=C(N(C=CC1(=O))C(OC(C2O)CO)C2O)N1</chem>	-1.98	-1.86	0.12	-1.84	0.14
guanosine	<chem>c1nc2C(=O)NC(N)=Nc2n1C3OC(CO)C(O)C3O</chem>	-1.90	-1.71	0.19	-2.06	-0.16
methionine	<chem>O=C(O)C(N)CCSC</chem>	-1.87	-2.41	-0.54	-1.85	0.02
ascorbic acid	<chem>O1C(=O)C(O)=C(O)C1C(O)CO</chem>	-1.85	-1.88	-0.03	-1.58	0.27
inosine	<chem>OCC1OC(C(O)C1O)n2cnc3C(=O)NC=Nc23</chem>	-1.85	-1.84	0.01	-1.87	-0.02
2,4,5,6(1H,3H)-pyrimidinetetrone	<chem>O=C(NC(=O)C(=O)C1(=O))N1</chem>	-1.84	-1.04	0.80	-0.85	0.99
urea, hydroxy-	<chem>NC(=O)NO</chem>	-1.80	-1.68	0.12	-1.83	-0.03
cytidine, 2-deoxy-	<chem>N1(C2OC(CO)C(O)C2)C(=O)N=C(N)C=C1</chem>	-1.77	-1.79	-0.02	-1.93	-0.16
1,2,3-propanetriol	<chem>OCC(O)CO</chem>	-1.76	-1.65	0.11	-1.93	-0.17
4H-imidazol-4-one, 2-amino-1,5-dihydro-1-methyl-	<chem>O=C(NC(=N)N1C)C1</chem>	-1.76	-1.21	0.55	-1.65	0.11
2(1H)-pyrimidinone, 4-amino-	<chem>N1C(=O)N=C(N)C=C1</chem>	-1.73	-1.47	0.26	-1.53	0.20
inosine, 2-deoxy-	<chem>OCC1OC(CC1O)n2cnc3C(=O)NC=Nc23</chem>	-1.71	-1.18	0.53	-1.67	0.04
isoleucine	<chem>O=C(O)C(N)C(CC)C</chem>	-1.70	-1.59	0.11	-1.73	-0.03
1,3-propanediol, 2,2-bis(hydroxymethyl)-	<chem>OCC(CO)(CO)CO</chem>	-1.69	-1.77	-0.08	-1.92	-0.23
acetamide, n-hydroxy-	<chem>CC(=O)NO</chem>	-1.59	-1.29	0.30	-1.46	0.13
6H-purin-6-one, 2-amino-1,9-dihydro-9-[(2-hydroxyethoxy)methyl]-	<chem>N1C(N)=Nc2n(COCCO)cnc2C1=O</chem>	-1.56	-1.70	-0.14	-1.45	0.11
leucine	<chem>O=C(O)C(N)CC(C)C</chem>	-1.52	-1.59	-0.07	-1.82	-0.30

formamide	O=CN	-1.51	-1.61	-0.10	-1.53	-0.02
uridine, 2-deoxy-	O=C(N(C=CC1(=O))C(OC(C2O)CO)C2)N1	-1.51	-1.19	0.32	-1.49	0.02
piperazine	N(CCNC1)C1	-1.50	-0.80	0.70	-1.16	0.34
1,3-propanediol, 2-ethyl-2-(hydroxymethyl)-	OCC(CC)(CO)CO	-1.48	0.19	1.67	-0.76	0.72
2,4,6(1H,3H,5H)-pyrimidinetrione	O=C(NC(=O)CC1(=O))N1	-1.47	-1.25	0.22	-1.12	0.35
riboflavin	Cc1c(C)cc2N=C3C(=O)NC(=O)N=C3N(CC(O)C(O)C(O)CO)c2c1	-1.46	-1.05	0.41	-1.05	0.41
glucose, 2-deoxy-2-[[[(methylnitrosoamino)carbonyl]amino]-phenylalanine	CN(N=O)C(=O)NC1C(O)OC(CO)C(O)C1O	-1.45	-1.61	-0.16	-1.71	-0.26
ethanol, 2,2-iminobis-	O=C(O)C(N)Cc(cccc1)c1	-1.44	-1.28	0.16	-1.35	0.09
1,4-piperazinedipropanamine	OCCNCCO	-1.43	-1.71	-0.28	-1.41	0.02
1,3-propanediamine	N(CCN(C1)CCCN)(C1)CCCN	-1.43	-1.35	0.08	-0.67	0.76
methane, sulfonylbis-	NCCCN	-1.43	-1.13	0.30	-1.41	0.02
1,2-benzenediol, 4-[1-hydroxy-2-(methylamino)ethyl]-	O=S(=O)(C)C	-1.41	-1.11	0.30	-0.95	0.46
1,3,5-triazine-2,4,6-triamine	OC(c(ccc(O)c1O)c1)CNC	-1.37	-0.69	0.68	-0.82	0.55
1,2-ethanediol	n(c(nc(n1)N)N)c1N	-1.37	-0.38	0.99	-0.69	0.68
methane, sulfinylbis-	OCCO	-1.36	-1.20	0.16	-1.53	-0.17
2,3-butanedione	O=S(C)C	-1.35	-1.22	0.13	-1.09	0.26
propanenitrile, 3,3-iminobis-	O=C(C(=O)C)C	-1.34	-1.34	0.00	0.07	1.41
ethanol, 2-amino-	C(#N)CCNCCC(#N)	-1.34	-1.15	0.19	-0.32	1.02
cytidine, 2,3-dideoxy-	OCCN	-1.31	-1.61	-0.30	-1.53	-0.22
guanosine, 2-deoxy-	O1C(CO)CCC1N2C(=O)N=C(N)C=C2	-1.30	-1.72	-0.42	-1.29	0.01
butanedioic acid, hydroxy-	O1C(CO)C(O)CC1n2c3N=C(N)NC(=O)c3nc2	-1.30	-1.04	0.26	-1.75	-0.45
galactopyranoside, 1-methylethyl 1-thioacetamide	O=C(O)CC(O)C(=O)O	-1.26	-1.68	-0.42	-0.87	0.39
1,2-benzenediol, 4-[2-amino-1-hydroxyethyl]-	O1C(CO)C(O)C(O)C(O)C1SC(C)C	-1.26	-1.25	0.01	-1.11	0.15
inosine, 2,3-dideoxy-	O=C(N)C	-1.26	-1.16	0.10	-1.10	0.16
glucopyranoside, 2-(hydroxymethyl)phenyl	c1cc(O)c(O)cc1C(O)CN	-1.24	-1.16	0.08	-1.40	-0.16
benzenesulfonamide, 4-amino-N-(aminoiminomethyl)-	O1C(CO)CCC1N2c3ncnc(O)c3N=C2	-1.24	-0.47	0.77	-0.99	0.25
1-naphthalenesulfonic acid, 2-amino-	O(C(CO)C(O)C1O)CO)C1O(c(ccc2)CO)c2	-1.22	-1.41	-0.19	-1.15	0.07
guanidine, cyano-	c1cc(N)ccc1S(=O)(=O)NC(=N)N	-1.22	-1.07	0.15	-0.55	0.67
6H-purin-6-one, 1,7-dihydro-	O=S(=O)(O)c(c(c(ccc1)cc2)c1)c2N	-1.16	-0.91	0.25	-0.75	0.41
acetic acid, hydroxy-	NC(=NC(#N))N	-1.15	-1.26	-0.11	-1.02	0.13
thiourea	N1C=Nc2nc[nH]c2C1(=O)	-1.11	-1.19	-0.08	-1.15	-0.04
2,4(1H,3H)-pyrimidinedione	O=C(O)CO	-1.11	-1.07	0.04	-1.02	0.09
tryptophan	NC(=S)N	-1.08	-1.31	-0.23	-1.07	0.01
adenosine	N1C(=O)NC(=O)C=C1	-1.07	-0.87	0.20	-1.20	-0.13
tryptophan	O=C(O)C(N)CC(c(c(N1)ccc2)c2)=C1	-1.06	-1.22	-0.16	-1.10	-0.04
acetamide, N-methyl-	n1cnc2n(C3OC(CO)C(O)C3(O))cnc2c1N	-1.05	-1.38	-0.33	-1.21	-0.16
1,3-propanediol	O=C(O)C(N)Cc(c(c(n1)ccc2)c2)c1	-1.05	-1.22	-0.17	-1.10	-0.05
3-quinolinecarboxylic acid, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-	O=C(NC)C	-1.05	-0.70	0.35	-1.06	-0.01
formamide, N,N-dimethyl-	OCCCO	-1.04	-0.71	0.33	-1.18	-0.14
ethanol, 2,2,2-nitritotris-	C1CNCCN1c2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2F	-1.03	-0.31	0.72	-0.47	0.56
uridine, 2,3-dideoxy-	O=CN(C)C	-1.01	-0.93	0.08	-0.77	0.24
butanedinitrile	OCCN(CCO)CCO	-1.00	-2.48	-1.48	-1.38	-0.38
formamide, N-methyl-	O1C(CO)CCC1N2C(=O)NC(=O)C=C2	-1.00	-1.12	-0.12	-1.06	-0.06
benzenepropanoic acid, beta-(aminomethyl)-4-chloro-	C(#N)CCC(#N)	-0.99	-0.63	0.36	-0.75	0.24
2-propanol, 1-amino-	O=CNC	-0.97	-1.14	-0.17	-1.31	-0.34
acetamide, N-[(4-aminophenyl)sulfonyl]-	c1cc(Cl)ccc1C(CN)CC(=O)O	-0.96	-1.32	-0.36	-0.82	0.14
oxiranemethanol	OC(CN)C	-0.96	-1.19	-0.23	-1.03	-0.07
2,5-pyrrolidinedione, 1-methyl-	O=C(NS(=O)(=O)c(ccc(N)c1)c1)C	-0.96	-0.60	0.36	0.15	1.11
ethanol, 2-(methylamino)-	O(C1CO)C1	-0.95	-1.09	-0.14	-0.93	0.02
propanenitrile, 3-hydroxy-	CN1C(=O)CCC1(=O)	-0.95	-0.64	0.31	-0.70	0.25
thymidine	OCCNC	-0.94	-1.15	-0.21	-1.05	-0.11
1,2-propanediol	C(#N)CCO	-0.94	-1.12	-0.18	-0.98	-0.04
	O=C(N(C=C(C1(=O))C)C(OC(C2O)C)O)C2)N1	-0.93	-0.64	0.29	-1.32	-0.39
	OCC(O)C	-0.92	-0.78	0.14	-1.10	-0.18

2,3-butanediol	OC(C(O)C)C	-0.92	-0.36	0.56	-0.59	0.33
6H-purin-6-one, 2-amino-1,7-dihydro-	N1C(N)=Nc2nc[nH]c2C1(=O)	-0.91	-1.05	-0.14	-0.97	-0.06
2-naphthacenecarboxamide, 4-(dimethylamino)-	O=C(N)C(=C(O)C(N(C)C)C(C1(O)C(O)=C(C2C(O)(c(c3c(O)cc4)c4)C)C3(=O))C2O)C1(=O)	-0.90	-2.87	-1.97	-0.99	-0.09
1,4,4a,5,5a,6,11,12a-octahydro-3,5,6,10,12,12a-hexahydroxy-6-methyl-1,11-dioxo-						
guanidine, nitro-	N(=O)(=O)NC(=N)N	-0.89	-1.72	-0.83	-0.97	-0.08
galactopyranoside, phenyl	O1C(CO)C(O)C(O)C(O)C1Oc2ccccc2	-0.89	-0.50	0.39	-0.64	0.25
glycine, N-(4-aminobenzoyl)-	O=C(NCC(=O)O)c(ccc(N)c1)c1	-0.89	-0.46	0.43	0.00	0.89
morpholine	O(CCNC1)C1	-0.86	-0.56	0.30	-0.75	0.11
1H-1,2,4-triazol-3-amine	n1nc(N)nc1	-0.86	-0.47	0.39	-0.89	-0.03
2-pyrrolidinone	O=C(NCC1)C1	-0.85	-0.32	0.53	-0.90	-0.05
3,6-pyridazinedione, 1,2-dihydro-	C1=CC(=O)NNC1(=O)	-0.84	-0.89	-0.05	-1.44	-0.60
1,4-butanediol	OCCCCO	-0.83	-0.22	0.61	-0.63	0.20
4-pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-	O=C1NC(=O)NC(C(=O)O)=C1	-0.83	-0.11	0.72	-0.89	-0.06
2-propanol, 1,1-iminobis-	OC(C)CNCC(O)C	-0.82	-0.88	-0.06	-0.40	0.42
propanedioic acid	O=C(O)CC(=O)O	-0.81	-1.25	-0.44	-0.60	0.21
2-butene-1,4-diol	OCC=CCO	-0.81	-0.43	0.38	-0.64	0.17
galactopyranoside, 2-nitrophenyl	N(=O)(=O)c1cccc1OC2C(O)C(O)C(O)C(CO)O2	-0.78	-0.68	0.10	-0.58	0.20
ethanol, 2-methoxy-	O(CCO)C	-0.77	-0.91	-0.14	-0.78	-0.01
methanol	OC	-0.77	-0.63	0.14	-1.38	-0.61
3,4-pyridinedimethanol, 5-hydroxy-6-methyl-	n(c(c(O)c(c1CO)CO)C)c1	-0.77	-0.56	0.21	-0.57	0.20
acetamide, N,N-dimethyl-	O=C(N(C)C)C	-0.77	-0.49	0.28	-0.59	0.18
thiophene, tetrahydro-, 1,1-dioxide	O=S(=O)(CCC1)C1	-0.77	-0.24	0.53	-0.65	0.12
acetic acid, cyano-	O=C(O)CC(#N)	-0.76	-0.76	0.00	-0.46	0.30
1H-purine-2,6-dione, 3,7-dihydro-	N1C(=O)Nc2nc[nH]c2C1(=O)	-0.73	-1.15	-0.42	-0.65	0.08
propanoic acid, 2-hydroxy-	O=C(O)C(O)C	-0.72	-0.65	0.07	-0.79	-0.07
4-pyridinecarboxylic acid, hydrazide	NNC(=O)c1ccncc1	-0.70	-0.81	-0.11	-0.71	-0.01
1H-imidazole-4-ethanamine	C1=NC=C(CCN)N1	-0.70	-0.73	-0.03	-0.88	-0.18
1,3-propanediol, 2-(bromomethyl)-2-(hydroxymethyl)-	OCC(CBr)(CO)CO	-0.70	0.04	0.74	-0.94	-0.24
1,4,7,10,13,16-hexaoxacyclooctadecane	O(CCOCCOCCOCCOCCOC1)C1	-0.68	-1.42	-0.74	-0.39	0.29
2-propenamide	O=C(N)C=C	-0.67	-0.81	-0.14	-0.65	0.02
2-imidazolidinethione	N(C(=S)NC1)C1	-0.66	-0.49	0.17	-1.07	-0.41
2H-1-benzopyran-2-one, 7-galactopyranosyloxy-4-methyl-	O=C(Oc(c(C(=O)C)ccc2OC(OC(C(O)C3O)CO)C3O)c2)C1	-0.66	-0.43	0.23	-0.34	0.32
phosphoric acid, trimethyl ester	O=P(OC)(OC)OC	-0.65	-0.60	0.05	-0.61	0.04
propanimidamide, 3-[[[2-[(aminoiminomethyl)amino]-4-thiazolyl]methyl]thio]-N-(aminosulfonyl)-	NS(=O)(=O)N=C(N)CCSCC1=CSC(N=C(N)N)=N1	-0.64	-0.65	-0.01	-0.20	0.44
2(3H)-furanone, dihydro-	O=C(OCC1)C1	-0.64	-0.31	0.33	-0.11	0.53
ethanol, 2,2-thiobis-	OCCSCCO	-0.63	-0.62	0.01	-0.65	-0.02
benzenesulfonamide, 4-amino-	O=S(=O)(N)c(ccc(N)c1)c1	-0.62	-0.55	0.07	-0.16	0.46
adenosine, 3-deoxy-	c12N=CN(C3OC(CO)CC3O)c1ncnc2N	-0.61	-0.91	-0.30	-0.85	-0.24
phosphonic acid, methyl-, dimethyl ester	O=P(OC)(OC)C	-0.61	-0.59	0.02	-0.58	0.03
propanedinitrile	C(#N)CC(#N)	-0.60	-0.60	0.00	-0.84	-0.24
thymidine, 3-deoxy-	O1C(CO)CCC1N2C(=O)NC(=O)C(C)=C2	-0.60	-0.58	0.02	-0.86	-0.26
butanedioic acid	O=C(O)CCC(=O)O	-0.59	-0.75	-0.16	-0.53	0.06
galactopyranoside, 4-nitrophenyl	O1C(CO)C(O)C(O)C(O)C1Oc2ccc(N(=O)=O)cc2	-0.59	-0.68	-0.09	-0.63	-0.04
5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]methyl]-8-oxo-7-[(1H-tetrazol-1-ylacetyl)amino]-1H-1,2,4-triazole	c1nnnn1CC(=O)NC2C(=O)N3C(C(=O)O)=C(CSc4nncc(C)s4)CSC23	-0.58	-2.19	-1.61	-0.40	0.18
methanamine	n1ncnc1	-0.58	-0.76	-0.18	-0.78	-0.20
adenosine, 2-deoxy-	NC	-0.57	-0.64	-0.07	-1.06	-0.49
	c1nc2c(N)ncnc2n1C3OC(CO)C(O)C3	-0.55	-0.71	-0.16	-0.95	-0.40
4H-pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-	c1nc(O)c2cnnc2n1	-0.55	-0.55	0.00	-0.41	0.14
ethanol, 2-(2-ethoxyethoxy)-	O(CCOCC)CCO	-0.54	-0.69	-0.15	-0.16	0.38
formic acid	O=CO	-0.54	-0.46	0.08	-0.47	0.07
acetamide, 2-chloro-	O=C(N)CCl	-0.53	-0.58	-0.05	-0.67	-0.14

1,4-butanediol, dimethanesulfonate	CS(=O)(=O)OCCCCOS(C)(=O)=O	-0.52	-0.68	-0.16	-0.90	-0.38
urea, dimethyl-	CNC(=O)NC	-0.49	-0.62	-0.13	-1.27	-0.78
pentanoic acid, 4-oxo-	O=C(O)CCCC(=O)C	-0.49	-0.49	0.00	-0.14	0.35
1,4,7,10,13-pentaoxacyclopentadecane	O(CCOCCOCCOCCOC1)C1	-0.48	-1.14	-0.66	-0.40	0.08
2-butenedioic acid	O=C(O)C=CC(=O)O	-0.48	0.05	0.53	0.21	0.69
4H-1-benzopyran-4-one, 7-[[2-o-(6-deoxy-alpha-l-mannopyranosyl)-d-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-1,3,5-trioxane	O4C(C)C(O)C(O)C(O)C4OC5C(O)C(O)C(CO)OC5Oc1cc(O)c2C(=O)CC(c3ccc(O)cc3)Oc2c1	-0.44	-0.52	-0.08	-0.24	0.20
2-propyn-1-amine	O(COC1)C1	-0.43	-0.56	-0.13	-0.95	-0.52
benzamide, 4-amino-	C(#C)CN	-0.43	-0.43	0.00	-0.72	-0.29
1,3-dioxolan-2-one, 4-methyl-	O=C(N)c(ccc(N)c1)c1	-0.41	-0.18	0.23	0.02	0.43
piperazine, 1,4-dimethyl-	O=C(OCC1C)O1	-0.41	0.08	0.49	0.13	0.54
2-propyn-1-ol	N(CCN(C1)C)(C1)C	-0.40	-0.38	0.02	-0.01	0.39
methanamine, N-methyl-	OCC#C	-0.38	-0.42	-0.04	-0.70	-0.32
2-pyrrolidinone, 1-methyl-	N(C)C	-0.38	-0.17	0.21	-0.53	-0.15
adenosine, 2-chloro-	O=C1CCCN1C	-0.38	-0.11	0.27	-0.72	-0.34
3-pyridinecarboxamide	c12ncn(C3OC(CO)C(O)C3O)c1nc(Cl)nc2N	-0.37	-0.73	-0.36	-0.28	0.09
1,3-dioxolane	O=C(N)c(cccn1)c1	-0.37	-0.45	-0.08	-0.45	-0.08
ethane, 1,1-oxybis[2-methoxy-]	O(CCO1)C1	-0.37	-0.31	0.06	-0.61	-0.24
propanoic acid, 2-hydroxy-2-methyl-	O(CCO)CCOC	-0.36	-0.48	-0.12	0.12	0.48
methane, nitro-	O=C(O)C(O)(C)C	-0.36	-0.20	0.16	-0.37	-0.01
2H-imidazole-2-thione, 1,3-dihydro-1-methyl-	N(=O)(=O)C	-0.35	-0.04	0.31	-0.17	0.18
acetaldehyde	S=C1NC=CN1C	-0.34	-0.49	-0.15	-0.38	-0.04
acetonitrile	O=CC	-0.34	-0.17	0.17	-0.01	0.33
1,3-benzenediamine	C(#N)C	-0.34	-0.15	0.19	-0.04	0.30
morpholine, 4-methyl-	Nc(cccc1N)c1	-0.33	-0.39	-0.06	0.01	0.34
ethanol, 2-methoxy-	O(CCN(C1)C)C1	-0.33	-0.35	-0.02	-0.14	0.19
hexanedinitrile	O(CCO)CC	-0.32	-0.42	-0.10	-0.28	0.04
ethanol	C(#N)CCCCC(#N)	-0.32	0.35	0.67	-0.14	0.18
1,4-benzenediamine	OCC	-0.31	-0.14	0.17	-0.40	-0.09
oxirane	Nc(ccc(N)c1)c1	-0.30	-0.39	-0.09	-0.01	0.29
uridine, 5-bromo-2-deoxy-	O(C1)C1	-0.30	-0.05	0.25	-0.47	-0.17
pentanedioic acid	C1=C(Br)C(=O)NC(=O)N1C2OC(CO)C(O)C2	-0.29	-0.80	-0.51	-0.97	-0.68
1H-pyrrole-2,5-dione	O=C(O)CCCC(=O)O	-0.29	-0.26	0.03	-0.25	0.04
butanedioic acid, 2,3-dihydroxy-, diethyl ester	N1C(=O)C=CC1(=O)	-0.29	-0.12	0.17	-0.78	-0.49
2,2-bioxirane	O=C(OCC)C(O)C(O)C(=O)OCC	-0.29	-0.08	0.21	-0.57	-0.28
2,5-hexanedione	C1OC1C2CO2	-0.28	-0.58	-0.30	-0.36	-0.08
1,4-dioxane	O=C(CCC(=O)C)C	-0.27	-0.81	-0.54	0.28	0.55
ethanethioamide	O(CCO)C1	-0.27	-0.32	-0.05	-0.23	0.04
acetamide, N-[5-(aminosulfonyl)-1,3,4-thiadiazol-2-yl]-	NC(=S)C	-0.26	-0.83	-0.57	-0.30	-0.04
pyrazine	CC(=O)Nc1nnc(S(=O)(=O)N)s1	-0.26	-0.72	-0.46	-0.39	-0.13
adenosine, 2,3-dideoxy-	n(ccnc1)c1	-0.26	-0.06	0.20	-0.29	-0.03
2-propanone	O1C(CO)CCC1N2c3ncnc(N)c3N=C2	-0.25	-0.65	-0.40	-0.53	-0.28
2-propenoic acid, 2-hydroxyethyl ester	O=C(C)C	-0.24	-0.24	0.00	-0.29	-0.05
ethane, 1,2-dimethoxy-	O=C(OCCO)C=C	-0.21	-0.25	-0.04	0.04	0.25
acetamide, 2-iodo-	O(CCO)C	-0.21	-0.21	0.00	0.03	0.24
ethanedioic acid, dimethyl ester	O=C(N)CI	-0.19	-0.08	0.11	-0.03	0.16
1,4-dithiin, 2,3-dihydro-5,6-dimethyl-, 1,1,4,4-tetraoxide	O=C(OC)C(=O)OC	-0.17	-0.58	-0.41	0.01	0.18
acetic acid	CC1=C(C)S(=O)(=O)CCS1(=O)=O	-0.17	0.04	0.21	-0.93	-0.76
5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[aminocarbonyl]oxy]methyl]-7-[[2-furanyl(methoxyimino)acetyl]amino]-8-oxo-	O=C(O)C	-0.17	0.09	0.26	-0.12	0.05
carbamic acid, ethyl ester	CON=C(C(=O)NC2C1SCC(=C(N1C2=O)C(O)=O)COC(N)=O)c3ccco3	-0.16	0.29	0.45	-0.24	-0.08
benzenesulfonic acid, hydrazide	O=C(OCC)N	-0.15	-0.02	0.13	-0.14	0.01
pentanoic acid, 4-oxo-, methyl ester	O=S(=O)(NN)c(cccc1)c1	-0.14	0.01	0.15	0.26	0.40
ethanamine	CC(=O)CCC(=O)OC	-0.13	-0.20	-0.07	-0.17	-0.04
propanamide, N,N-dimethyl-	NCC	-0.13	-0.15	-0.02	-0.20	-0.07
1H-purin-6-amine	O=C(N(C)C)CC	-0.11	0.01	0.12	-0.06	0.05
benzenesulfonamide, 4-amino-N-2-pyrimidinyl-	n(c(c(ncn1)c1n2)N)c2	-0.09	-0.73	-0.64	-0.38	-0.29
1H-imidazole	n1c(NS(=O)(=O)c2ccc(N)cc2)nccc1	-0.09	-0.34	-0.25	0.25	0.34
6H-purine-6-thione, 2-amino-1,7-dihydro-	N1C=NC=C1	-0.08	0.06	0.14	-0.21	-0.13
2H-1,2,4-benzothiadiazine-7-sulfonamide, 6-chloro-	N1C(N)=Nc2ncnc2C1=S	-0.07	-0.31	-0.24	-0.73	-0.66
	O=S(=O)	-0.07	-0.10	-0.03	-0.16	-0.09

3,4-dihydro-, 1,1-dioxide	(N)c(c(cc(NCNS1(=O)=O)c12)Cl)c2					
1H-imidazole, 1-methyl-	N(C=CN1C)=C1	-0.06	0.61	0.67	-0.18	-0.12
propanedioic acid, dimethyl ester	O=C(OC)CC(=O)OC	-0.05	-0.09	-0.04	0.08	0.13
2-pyrrolidinone, 1-ethyl-	O=C(N(CC1)CC)C1	-0.04	0.38	0.42	0.13	0.17
2-oxazolidinone, 3-[[[(5-nitro-2-furanyl)methylene]amino]-	O=C(OCC1)N1N=Cc(oc(N=O)(=O))c2	-0.04	1.02	1.06	0.49	0.53
2-naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-	CC3C2C(O)C1C(N(C)C)C(=C(C(N)=O)C(=O)C1(O)C(=C2C(=O)c4c(O)cc(c34)O)O	-0.02	-1.36	-1.34	-0.72	-0.70
1H-purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-	CN1C(=O)N(C)c2ncnc2C1(=O)	-0.02	-0.39	-0.37	-0.26	-0.24
1H-imidazole-1-ethanol, 2-methyl-5-nitro-	Cc1ncc(N(=O)=O)n1CCO	-0.02	0.00	0.02	-0.15	-0.13
5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[(aminocarbonyl)oxy]methyl]-7-methoxy-8-oxo-7-[(2-thienylacetyl)amino]-	COC3(NC(=O)Cc1cccs1)C2SCC(=C(N2C3=O)C(O)=O)COC(N)=O	-0.02	0.22	0.24	0.22	0.24
2-propenal	O=CC=C	-0.01	0.19	0.20	0.18	0.19
methane, dimethoxy-	O(COC)C	0.00	-0.19	-0.19	-0.37	-0.37
6H-purine-6-thione, 1,7-dihydro-	n1cnc2ncnc2c1S	0.01	-0.13	-0.14	0.04	0.03
formic acid, methyl ester	O=COC	0.03	-0.17	-0.20	-0.31	-0.34
ethanol, 2-chloro-	OCCCl	0.03	0.11	0.08	0.00	-0.03
2-propen-1-amine	NCC=C	0.03	0.21	0.18	-0.43	-0.46
oxirane, methyl-	O(C1C)C1	0.03	0.37	0.34	0.04	0.01
phenol, 4-amino-	Oc(ccc(N)c1)c1	0.04	0.24	0.20	0.47	0.43
ethanol, 2-(1-methylethoxy)-	O(C(C)C)CCO	0.05	0.00	-0.05	0.06	0.01
thymidine, 3-azido-3-deoxy-	C1=C(C)C(=O)NC(=O)N1C2OC(CO)C(N=N#N)C2	0.05	0.23	0.18	-0.10	-0.15
2-propanol	OC(C)C	0.05	0.28	0.23	0.04	-0.01
benzenesulfonamide, 4-amino-N-2-thiazolyl-	c1cc(N)ccc1S(=O)(=O)Nc2nccs2	0.05	0.72	0.67	0.88	0.83
heptanedinitrile	C(#N)CCCCC(#N)	0.05	0.84	0.79	0.29	0.24
ethanedinitrile	C(#N)C(#N)	0.07	0.07	0.00	-0.65	-0.72
acetamide, N-(4-aminophenyl)-	O=C(Nc(ccc(N)c1)c1)C	0.08	0.18	0.10	0.14	0.06
isoxazole	n1occc1	0.08	0.21	0.13	0.38	0.30
hexanedioic acid	O=C(O)CCCCC(=O)O	0.08	0.23	0.15	0.13	0.05
benzamide, N-(1-methylethyl)-4-[(2-methylhydrazino)methyl]-	CNNCc1ccc(cc1)C(=O)NC(C)C	0.08	1.29	1.21	0.53	0.45
4H-pyran-4-one, 3-hydroxy-2-methyl-	O1C(C)=C(O)C(=O)C=C1	0.09	-0.19	-0.28	-0.24	-0.33
acetic acid, mercapto-	O=C(O)CS	0.09	0.03	-0.06	0.09	0.00
thiourea, trimethyl-	N(C(N(C)C)=S)C	0.10	-0.17	-0.27	0.08	-0.02
1H-purine, 6-[(1-methyl-4-nitro-1H-imidazol-5-yl)thio]-	N(=O)c1cncn(C)c1Sc2ncnc3ncnc23	0.10	-0.09	-0.19	0.84	0.74
methane, oxybis-	O(C)C	0.10	0.07	-0.03	-0.16	-0.26
3-pyridinamine	n(cccc1N)c1	0.11	-0.11	-0.22	0.18	0.07
2-pyridineethanol	n(c(ccc1)CCO)c1	0.12	0.38	0.26	0.45	0.33
1,3-benzenediamine, 4-methyl-	Nc(c(ccc1N)C)c1	0.14	0.16	0.02	0.37	0.23
benzenesulfonamide, 4-amino-N-(4-methyl-2-pyrimidinyl)-	O=S(=O)(Nc(nccc1C)n1)c(ccc(N)c2)c2	0.14	0.21	0.07	0.44	0.30
1,2-benzenediamine	Nc(c(N)ccc1)c1	0.15	0.16	0.01	-0.08	-0.23
benzeneacetamide, 4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-	CC(C)NCC(O)COc1ccc(CC(=O)(N))cc1	0.16	-0.03	-0.19	0.57	0.41
methanamine, N,N-dimethyl-	N(C)(C)C	0.16	0.04	-0.12	-0.14	-0.30
propanenitrile	C(#N)CC	0.16	0.35	0.19	-0.01	-0.17
1,3,5-benzenetriol	Oc(cc(O)cc1O)c1	0.16	0.55	0.39	0.25	0.09
2-propen-1-ol	OCC=C	0.17	0.21	0.04	-0.03	-0.20
acetic acid, methyl ester	O=C(OC)C	0.18	0.37	0.19	0.18	0.00
ethane, nitro-	N(=O)(=O)CC	0.18	0.45	0.27	0.45	0.27
propanenitrile, 3-chloro-	C(#N)CCCl	0.18	0.60	0.42	0.41	0.23
urea, tetramethyl-	O=C(N(C)C)N(C)C	0.19	-0.20	-0.39	-0.06	-0.25
ethanone, 1-pyrazinyl-	O=C(c(nccn1)c1)C	0.20	-0.38	-0.58	-0.15	-0.35
2,5-cyclohexadiene-1,4-dione	O=C1C=CC(=O)C=C1	0.20	0.25	0.05	0.21	0.01
phenol, 3-amino-	Oc(cccc1N)c1	0.21	0.24	0.03	0.43	0.22
pyrazine, methyl-	n(ccnc1C)c1	0.21	0.49	0.28	0.19	-0.02
acetic acid, chloro-	O=C(O)CCl	0.22	0.34	0.12	0.18	-0.04
adenosine, N-benzoyl-2-deoxy-	O1C(CO)C(O)CC1N2c3ncnc(NC(=O)c4ccccc4)c3N=C2	0.22	0.69	0.47	0.29	0.07
2-butenedioic acid, dimethyl ester	O=C(OC)C=CC(=O)OC	0.22	1.21	0.99	0.45	0.23
hydrazinecarboxamide, 2-[(5-nitro-2-furanyl)methylene]-	O=C(N)NN=Cc(oc(N(=O)(=O))c1)c1	0.23	0.23	0.00	0.23	0.00
formic acid, ethyl ester	O=COCC	0.23	0.32	0.09	0.38	0.15

methanesulfonamide, N-[4-[1-hydroxy-2-[(1-methylethyl)amino]ethyl]phenyl]-	<chem>c1cc(S(=O)(=O)C)ccc1C(O)CNC(C)C</chem>	0.24	-0.26	-0.50	0.19	-0.05
gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1-alpha,2,4a-alpha,4b,10)-	<chem>O=C(OC(C1C(C2(CC(O)(C3=C)CC4)C3)C(=O)O)(C24)C=CC5O)C15C</chem>	0.24	0.45	0.21	0.66	0.42
1H-imidazole, 2-methyl-	<chem>N(C=CN1)=C1C</chem>	0.24	0.61	0.37	0.36	0.12
butanoic acid, 3-oxo-, ethyl ester	<chem>O=C(OC)CC(=O)C</chem>	0.25	-0.20	-0.45	0.19	-0.06
methane, trimethoxy-	<chem>O(C(OC)OC)C</chem>	0.25	-0.03	-0.28	-0.23	-0.48
2-propenenitrile	<chem>C(#N)C=C</chem>	0.25	0.21	-0.04	0.20	-0.05
1-propanol	<chem>OCCC</chem>	0.25	0.35	0.10	0.21	-0.04
1,2,3-propanetriol, triacetate	<chem>O=C(OC(OC(=O)C)COC(=O)C)C</chem>	0.25	0.36	0.11	0.40	0.15
4-pyridinamine	<chem>n(ccc(N)c1)c1</chem>	0.26	-0.11	-0.37	0.08	-0.18
2-propanamine	<chem>NC(C)C</chem>	0.26	0.27	0.01	-0.05	-0.31
benzamide, N-hydroxy-	<chem>O=C(NO)c(cccc1)c1</chem>	0.26	0.61	0.35	0.17	-0.09
3-butyne-2-ol, 2-methyl-	<chem>OC(C#C)(C)C</chem>	0.28	0.45	0.17	0.08	-0.20
2-furanmethanol	<chem>C1=C(CO)OC=C1</chem>	0.28	0.45	0.17	0.25	-0.03
2-butanone	<chem>O=C(CC)C</chem>	0.29	0.26	-0.03	0.41	0.12
1,2-ethanediamine, N,N,N,N-tetramethyl-	<chem>N(CCN(C)C)(C)C</chem>	0.30	-0.26	-0.56	0.33	0.03
benzenesulfonamide	<chem>O=S(=O)(N)c(cccc1)c1</chem>	0.31	0.37	0.06	0.32	0.01
1H-imidazole, 1,2-dimethyl-5-nitro-	<chem>Cc1ncc(N(=O)=O)n1C</chem>	0.31	0.97	0.66	-0.01	-0.32
4-pyridinecarboxylic acid	<chem>O=C(O)c(ccnc1)c1</chem>	0.32	0.69	0.37	0.28	-0.04
propanoic acid	<chem>O=C(O)CC</chem>	0.33	0.58	0.25	0.31	-0.02
benzeneacetic acid, 4-hydroxy-3-methoxy-	<chem>O=C(O)Cc(ccc(O)c1OC)c1</chem>	0.33	0.77	0.44	1.02	0.69
acetamide, N,N-diethyl-	<chem>O=C(N(CC)CC)C</chem>	0.34	0.50	0.16	0.50	0.16
L-proline, 1-(3-mercapto-2-methyl-1-oxopropyl)-	<chem>CC(CS)C(=O)N1CCCC1C(=O)(O)</chem>	0.34	0.84	0.50	1.02	0.68
2-propenoic acid, 2-hydroxypropyl ester	<chem>O=C(OC(C)O)C=C</chem>	0.35	0.17	-0.18	0.40	0.05
formaldehyde	<chem>O=C</chem>	0.35	0.35	0.00	-0.68	-1.03
butanedioic acid, dimethyl ester	<chem>O=C(OC)CCC(=O)OC</chem>	0.35	0.40	0.05	0.20	-0.15
2-propenoic acid	<chem>O=C(O)C=C</chem>	0.35	0.44	0.09	0.46	0.11
2-propanol, 2-methyl-	<chem>OC(C)(C)C</chem>	0.35	0.73	0.38	0.70	0.35
pyrimidine, 2-chloro-	<chem>C1=CN=C(Cl)N=C1</chem>	0.36	0.58	0.22	0.86	0.50
3-pyridinecarboxylic acid	<chem>O=C(O)c(cccn1)c1</chem>	0.36	0.69	0.33	0.29	-0.07
2-pyrrolidinone, 1-ethenyl-	<chem>O=C(N(C=C)CC1)C1</chem>	0.37	0.25	-0.12	-0.11	-0.48
2-furanmethanamine	<chem>C1=C(CN)OC=C1</chem>	0.37	0.44	0.07	-0.43	-0.80
ethyne	<chem>C#C</chem>	0.37	0.50	0.13	-0.03	-0.40
2,5-pyrrolidinedione, 3-ethyl-3-methyl-	<chem>CCC1(C)CC(=O)NC1=O</chem>	0.38	0.51	0.13	0.10	-0.28
3H-pyrazol-3-one, 1,2-dihydro-1,5-dimethyl-2-phenyl-	<chem>c1ccccc1N2C(=O)C=C(C)N2C</chem>	0.38	0.59	0.21	1.18	0.80
2-thiazolamine	<chem>s1c(N)ncc1</chem>	0.38	0.83	0.45	0.33	-0.05
ethane, 1,1-oxybis[2-ethoxy-]	<chem>O(CCOCC)CCOCC</chem>	0.39	0.50	0.11	0.64	0.25
2,4-pentanedione	<chem>O=C(CC(=O)C)C</chem>	0.40	0.05	-0.35	-0.20	-0.60
guanidine, N-cyano-N-methyl-N-[2-[[[(5-methyl-1H-imidazol-4-yl)methyl]thio]ethyl]-	<chem>CNC(NCCSCC1NC=NC=1C)=NC(#N)</chem>	0.40	0.57	0.17	0.42	0.02
2-propanamine, 2-methyl-	<chem>NC(C)(C)C</chem>	0.40	0.72	0.32	0.81	0.41
guanidine, N,N,N,N-tetramethyl-	<chem>N=C(N(C)C)N(C)C</chem>	0.41	-0.28	-0.69	-0.23	-0.64
ethanol, 2,2,2-trifluoro-	<chem>FC(F)(F)CO</chem>	0.41	0.27	-0.14	0.61	0.20
2-furancarboxaldehyde	<chem>O=CC(OC=C1)=C1</chem>	0.41	0.83	0.42	0.43	0.02
ethanone, 1-(3-pyridinyl)-	<chem>O=C(c(cccn1)c1)C</chem>	0.43	0.49	0.06	0.45	0.02
4-pyridinecarboxaldehyde	<chem>O=Cc(ccnc1)c1</chem>	0.43	0.52	0.09	0.16	-0.27
propanoic acid, 3-mercapto-	<chem>O=C(O)CCS</chem>	0.43	0.52	0.09	0.34	-0.09
2-pyridinecarboxaldehyde	<chem>O=Cc(nccc1)c1</chem>	0.44	0.52	0.08	0.54	0.10
thiazole	<chem>s1cncc1</chem>	0.44	0.99	0.55	0.89	0.45
7-oxabicyclo[4.1.0]heptane, 3-oxiranyl-	<chem>O(C1C(CC(O2)C2C3)C3)C1</chem>	0.44	1.13	0.69	0.85	0.41
2-pyridinecarbonitrile	<chem>C(#N)c(nccc1)c1</chem>	0.45	0.35	-0.10	0.59	0.14
oxirane, (chloromethyl)-	<chem>O(C1CC1)C1</chem>	0.45	0.63	0.18	0.35	-0.10
phosphonic acid, bis(1-methylethyl) ester	<chem>O=P(OC(C)C)OC(C)C</chem>	0.45	0.68	0.23	0.93	0.48
acetamide, N-(4-hydroxyphenyl)-	<chem>O=C(Nc(ccc(O)c1)c1)C</chem>	0.46	0.27	-0.19	0.51	0.05
pyrrolidine	<chem>N(CCC1)C1</chem>	0.46	0.70	0.24	0.16	-0.30
propanenitrile, 2-methyl-	<chem>N#CC(C)C</chem>	0.46	0.76	0.30	0.50	0.04
furan, tetrahydro-	<chem>O(CCC1)C1</chem>	0.46	0.94	0.48	0.35	-0.11
2-propenoic acid, 2-methyl-, 2-hydroxyethyl ester	<chem>O=C(OC(C)C)C(=O)C</chem>	0.47	0.30	-0.17	0.27	-0.20
benzenesulfonamide, N-hydroxy-	<chem>O=S(=O)(NO)c(cccc1)c1</chem>	0.48	0.25	-0.23	0.28	-0.20
1-propanamine	<chem>NCCC</chem>	0.48	0.34	-0.14	0.31	-0.17
ethanamine, N-ethyl-N-nitroso-	<chem>O=NN(CC)CC</chem>	0.48	0.34	-0.14	0.60	0.12
2-pyridinamine	<chem>n(c(N)ccc1)c1</chem>	0.48	0.53	0.05	0.42	-0.06
thiourea, tetramethyl-	<chem>N(C(N(C)C)=S)(C)C</chem>	0.49	0.04	-0.45	0.35	-0.14
pyrimidine, 2-(1-piperazinyl)-	<chem>n1ccccc1N2CCNCCC2</chem>	0.49	0.35	-0.14	0.32	-0.17

1-propanol, 3-chloro-phosphonic acid, (2,2,2-trichloro-1-hydroxyethyl)-, dimethyl ester	OCCCCI COP(=O)(OC)C(O)C(Cl)(Cl)Cl	0.50 0.51	0.60 -0.28	0.10 -0.79	0.36 0.81	-0.14 0.30
ethanone, 1-(2-furanyl)-benzenesulfonamide, N-(phenylsulfonyl)-	O=C(C(OC=C1)=C1)C O=S(=O)(NS(=O)(=O)c(cccc1)c1)c(cccc2)c2	0.52 0.52	0.80 1.16	0.28 0.64	0.73 1.72	0.21 1.20
1,4-benzenediamine, 2-nitro-butanenitrile	N(=O)(=O)c(c(N)ccc1N)c1 C(#N)CCC	0.53 0.53	0.55 0.84	0.02 0.31	1.00 0.59	0.47 0.06
ethanone, 1,2-di-2-furanyl-2-hydroxy-	O=C(C(OC=C1)=C1)C(O)C(OC=C2)=C2	0.54	0.33	-0.21	0.80	0.26
pyrazine, 2,3-dimethyl-erythro-alpha-galacto-octopyranoside, methyl 6,8-dideoxy-6-[[[1-methyl-4-propyl-2-pyrrolidinyl]carbonyl]amino]-1-thio-ethanol, 2-(2-butoxyethoxy)-ethanedioic acid, diethyl ester	n(c(c(nc1)C)C)c1 CCCC1CC(N(C)C1)C(=O)NC(C(C)O)C2OC(SC)C(O)C(O)C2O	0.54 0.56	1.03 0.29	0.49 -0.27	0.63 0.50	0.09 -0.06
2-propanol, 1-methoxy-, acetate	O(CCOCCO)CCCC O=C(OCC)C(=O)OCC	0.56 0.56	0.29 0.40	-0.27 -0.16	0.63 1.15	0.07 0.59
thiourea, N,N-diethyl-benzamide, 5-(aminosulfonyl)-N-[(1-ethyl-2-pyrrolidinyl)methyl]-2-methoxy-ethanamine, N-ethyl-benzenesulfonamide, N,4-dimethyl-N-nitroso-propanal	COCC(OC(=O)C)C N(C(=S)NCC)CC CCN1CCCC1CNC(=O)c2cc(ccc2OC)S(N)(=O)=O N(CC)CC O=S(=O)(N(N=O)C)c(ccc(c1)C)c1	0.56 0.57 0.57 0.58 0.58 0.59	0.52 0.60 0.65 0.81 0.92	-0.04 0.03 0.08 0.23 0.34	0.77 0.62 1.20 0.76 1.14	0.21 0.05 0.63 0.18 0.56
1,4-benzenediol	O=CCC Oc(ccc(O)c1)c1	0.59 0.59	0.33 1.03	-0.26 0.44	0.31 0.71	-0.28 0.12
furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-6(5aH)-one, 9-[[4,6-o-ethylidene-beta-glucopyranosyl]oxy]-5,8,8a,9-tetrahydro-5-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-propanediol, 3-(2-methoxyphenoxy)-, 1-carbamate	O1C2COC(C)OC2C(O)C(O)C1OC3C4COC(=O)C4C(c5cc(OC)c(O)c(OC)c5)c6cc7OCOc7cc36 O=C(OCC(O)COc(c(OC)ccc1)c1)N	0.60 0.61	0.04 -0.26	-0.56 -0.87	0.73 0.63	0.13 0.02
heptanedioic acid	O=C(O)CCCCC(=O)O	0.61	0.72	0.11	0.51	-0.10
2-butanol	OC(CC)C	0.61	0.77	0.16	0.66	0.05
benzeneacetic acid, alpha-hydroxy-phenol, 2-amino-pentanedioic acid, dimethyl ester	O=C(O)C(O)c(cccc1)c1 Oc(c(N)ccc1)c1 O=C(OC)CCCC(=O)OC	0.62 0.62 0.62	0.57 0.60 0.90	-0.05 -0.02 0.28	0.66 0.35 0.59	0.04 -0.27 -0.03
glucose, 2,3,4,5,6-pentaacetate	O=C(OCC(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C1OC(=O)C	0.63	-0.79	-1.42	0.41	-0.22
glucopyranose, pentaacetate	CC(=O)OCC1OC(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C1OC(=O)C	0.63	-0.75	-1.38	0.53	-0.10
2-naphthalenesulfonic acid	O=S(=O)(O)c(ccc(c1ccc2)c2)c1	0.63	0.01	-0.62	-0.38	-1.01
4H-pyran-4-one, 2-ethyl-3-hydroxy-2H-1,3,2-oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide	O1C(CC)=C(O)C(=O)C=C1 C1CCNP(=O)(N(CCCl)CCCl)O1	0.63 0.63	0.30 0.97	-0.33 0.34	0.34 0.76	-0.29 0.13
pyrazine, 2,5-dimethyl-oxirane, (butoxymethyl)-2-butanone, oxime	n(c(cnc1C)C)c1 O(C1COCCCC)C1 N(O)=C(CC)C	0.63 0.63 0.63	1.03 1.08 1.69	0.40 0.45 1.06	0.62 1.18 0.86	-0.01 0.55 0.23
methane, trifluoro-benzamide	FC(F)F O=C(N)c(cccc1)c1	0.64 0.64	0.58 0.74	-0.06 0.10	0.97 0.51	0.33 -0.13
5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[aminophenylacetyl]amino]-3-methyl-8-oxo-2,4,6(1H,3H,5H)-pyrimidinetrione, 5,5-diethyl-benzenecarboximidamide	CC1=C(N3C(SC1)C(NC(=O)C(N)c2ccccc2)C3=O)C(O)=O CCC1(CC)C(=O)NC(=O)NC1(=O)c1cccc1C(=N)N	0.65 0.65	0.40 0.75	-0.25 0.10	0.55 0.73	-0.10 0.08
pyridine	cccc1c1	0.65	0.80	0.15	0.70	-0.37
benzoic acid, 3-amino-cytidine, N-benzoyl-2-deoxy-	O=C(O)c(cccc1N)c1 O1C(CO)C(O)CC1N2C(=O)N=C(NC(=O)c3ccccc3)C=C2	0.65 0.67	0.96 0.05	0.31 -0.62	0.93 -0.09	0.28 -0.76
1H-indene-1,3(2H)-dione, 2,2-dihydroxy-1,3,5-trioxane, 2,4,6-trimethyl-2-furancarboxaldehyde, 5-methyl-2-pyridineethanamine, N-methyl-2H-pyran, 3,4-dihydro-benzenesulfonamide, 4-amino-N-(5,6-dimethoxy-4-pyrimidinyl)-ethanamine, N,N-dimethyl-benzoic acid, 3,4,5-trihydroxy-1,3-propanediol, 2-methyl-2-propyl-, dicarbamate	O=C(c(c(C1(=O))ccc2)c2)C1(O)O O(C(OC(O1)C)C)C1C O=CC(OC(=C1)C)=C1 n(c(ccc1)CCNC)c1 O(C=CCC1)C1 c1cc(N)ccc1S(=O)(=O)Nc2c(OC)c(OC)ncn2 N(CC)(C)C O=C(O)c(cc(O)c(O)c1O)c1 O=C(OCC(CCC)C)COC(=O)N)N NC(=S)Nc(cccc1)c1	0.67 0.67 0.67 0.68 0.69 0.70 0.70 0.70 0.71	0.32 0.70 1.38 0.48 1.21 -0.24 0.53 0.86 0.98 0.95	-0.35 0.03 0.71 -0.20 0.52 -0.94 -0.17 0.16 0.28 0.24	0.84 0.33 0.69 0.59 1.40 0.72 0.71 1.17 1.06 0.57	0.17 -0.34 0.02 -0.09 0.71 0.02 0.01 0.47 0.36 -0.14

2-pyridinecarboxylic acid	<chem>O=C(O)c1cccc1c1</chem>	0.72	0.69	-0.03	0.22	-0.50
pyrimidine, 5-bromo-	<chem>n(cc(Br)cn1)c1</chem>	0.72	0.83	0.11	0.66	-0.06
2-butenic acid	<chem>O=C(O)C=CC</chem>	0.72	0.85	0.13	0.94	0.22
acetic acid ethenyl ester	<chem>O=C(OC=C)C</chem>	0.73	0.73	0.00	0.83	0.10
1-propanamine, 2-methyl-	<chem>NCC(C)C</chem>	0.73	0.76	0.03	0.54	-0.19
acetic acid ethyl ester	<chem>O=C(OCC)C</chem>	0.73	0.86	0.13	0.74	0.01
pyrazine, methoxy-	<chem>O(c1cccn1)c1C</chem>	0.73	0.92	0.19	0.59	-0.14
1,2-benzenedicarboxylic acid	<chem>O=C(O)c1c(ccc1)C(=O)O)c1</chem>	0.73	1.07	0.34	1.22	0.49
2-butanamine	<chem>NC(CC)C</chem>	0.74	0.76	0.02	0.79	0.05
1H-pyrrole	<chem>C1=CC=CN1</chem>	0.75	0.88	0.13	0.76	0.01
1,2-benzenedicarboxylic acid, 3-nitro-	<chem>O=C(O)c1c(c(N(=O)(=O))cc1)C(=O)O)c1</chem>	0.75	0.89	0.14	1.11	0.36
benzeneacetic acid, 4-hydroxy-	<chem>O=C(O)Cc1ccc(O)c1c1</chem>	0.75	0.95	0.20	0.93	0.18
ethane, 1,1-difluoro-	<chem>FC(F)C</chem>	0.75	1.13	0.38	0.79	0.04
1-propanol, 2-methyl-	<chem>OCC(C)C</chem>	0.76	0.77	0.01	0.60	-0.16
benzeneacetic acid, alpha-(hydroxymethyl)-	<chem>O=C(O)C(c1cccc1)c1CO</chem>	0.77	0.38	-0.39	0.77	0.00
4-pyridinecarboxaldehyde, oxime	<chem>ON=Cc1ccncc1</chem>	0.77	0.68	-0.09	0.12	-0.65
butanoic acid	<chem>O=C(O)CCC</chem>	0.79	1.07	0.28	0.78	-0.01
1(3H)-isobenzofuranone	<chem>O=C(OC1CCCC2)c12</chem>	0.80	0.71	-0.09	0.99	0.19
2-propenoic acid, methyl ester	<chem>O=C(OC)C=C</chem>	0.80	0.73	-0.07	0.67	-0.13
phosphoric acid, triethyl ester	<chem>OP(=O)(OCC)OCC</chem>	0.80	0.87	0.07	0.71	-0.09
1,3-benzenediol	<chem>Oc1ccc(O)c1</chem>	0.80	1.03	0.23	0.70	-0.10
cyclohexanone	<chem>O=C1CCCCC1C1</chem>	0.81	1.13	0.32	1.03	0.22
2,3-naphthalenediol, 5-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]-1,2,3,4-tetrahydro-	<chem>CC(C)C1NCC(O)COc1cccc2CC(O)C(O)Cc12</chem>	0.81	1.17	0.36	1.23	0.42
benzamide, 4-nitro-	<chem>O=C(N)c1ccc(N(=O)(=O))c1c1</chem>	0.82	0.56	-0.26	0.31	-0.51
ethanol, 2-(phenylamino)-	<chem>OCCNc1cccc1c1</chem>	0.82	0.65	-0.17	0.73	-0.09
benzenesulfonamide, 4-methyl-	<chem>O=S(=O)(N)c1ccc(C)C1</chem>	0.82	0.92	0.10	0.72	-0.10
1H-indole-2,3-dione	<chem>O=C(Nc1ccc2c2)C1(=O)</chem>	0.83	0.45	-0.38	0.89	0.06
ethanol, 2-butoxy-	<chem>O(CCCC)CCO</chem>	0.83	0.57	-0.26	0.78	-0.05
3-pyridinecarboxylic acid, methyl ester	<chem>O=C(OC)c1cccn1c1</chem>	0.83	0.64	-0.19	0.45	-0.38
urea, phenyl-	<chem>O=C(Nc1cccc1c1)N</chem>	0.83	0.71	-0.12	0.85	0.02
ethanone, 1-(4-aminophenyl)-	<chem>O=C(c1ccc(N)c1)c1C</chem>	0.83	0.76	-0.07	1.31	0.48
formic acid, propyl ester	<chem>O=COCCC</chem>	0.83	0.81	-0.02	0.93	0.10
benzoic acid, 4-amino-	<chem>O=C(O)c1ccc(N)c1c1</chem>	0.83	0.96	0.13	0.78	-0.05
2-butanone, 3-methyl-	<chem>O=C(C(C)C)C</chem>	0.84	0.67	-0.17	0.78	-0.06
propanoic acid, methyl ester	<chem>O=C(OC)CC</chem>	0.84	0.86	0.02	0.68	-0.16
cyclohexanone, oxime	<chem>N(O)=C1CCCCC1C1</chem>	0.84	0.91	0.07	1.52	0.68
benzenesulfonamide, 2-methyl-	<chem>O=S(=O)(N)c1ccc(C)C1</chem>	0.84	0.92	0.08	0.61	-0.23
piperidine	<chem>N1CCCCC1C1</chem>	0.84	1.19	0.35	0.97	0.13
ethane, 1,1-diethoxy-	<chem>O(C1OCC)C1CC</chem>	0.84	1.20	0.36	1.19	0.35
ethanone, 1-(2-pyridinyl)-	<chem>O=C(c1cccn1)c1C</chem>	0.85	0.49	-0.36	0.69	-0.16
benzeneacetic acid, 3-hydroxy-	<chem>OC(=O)Cc1cc(O)ccc1</chem>	0.85	0.95	0.10	0.93	0.08
benzenesulfonamide, 2-chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1H-isindol-1-yl)-	<chem>NS(=O)(=O)c1cc(ccc1Cl)C2(O)NC(=O)c3cccc23</chem>	0.85	1.01	0.16	1.27	0.42
1-butanol, 4-chloro-	<chem>CCCCCl</chem>	0.85	1.10	0.25	0.97	0.12
1,3,5-triazine, hexahydro-1,3,5-trinitro-	<chem>N(=O)(=O)N(CN(N(=O)(=O))C1(=O))CN1N(=O)(=O)C1</chem>	0.87	0.68	-0.19	1.07	0.20
2-pyridinecarboxylic acid, ethyl ester	<chem>O=C(OCC)c1cccn1c1</chem>	0.87	0.82	-0.05	1.32	0.45
propane, 1-nitro-	<chem>N(=O)(=O)CCC</chem>	0.87	0.95	0.08	0.91	0.04
4-thia-1-azobicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[amino(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-	<chem>c1cc(O)ccc1C(N)C(=O)NC2C(=O)N3C(C(=O)O)C(C)(C)SC23</chem>	0.87	0.97	0.10	0.75	-0.12
1,2-benzenediamine, 4-nitro-	<chem>N(=O)(=O)c1ccc(Nc1N)c1</chem>	0.88	0.55	-0.33	0.84	-0.04
butanal	<chem>O=CCCC</chem>	0.88	0.82	-0.06	1.10	0.22
1-butanol	<chem>CCCCC</chem>	0.88	0.84	-0.04	0.84	-0.04
1,2-benzenediol	<chem>Oc1c(O)ccc1c1</chem>	0.88	1.03	0.15	0.74	-0.14
benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)-	<chem>Cc1cc(NS(=O)(=O)c2ccc(N)cc2)no1</chem>	0.89	0.48	-0.41	0.79	-0.10
morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl- (5-alpha,6-alpha)-	<chem>C1=CC2C(N(C)C5)Cc3ccc(O)c4c3C2(C5)C(O4)C1O</chem>	0.89	0.72	-0.17	0.99	0.10
benzenesulfonamide, 4-amino-N-(4,6-dimethyl-2-pyrimidinyl)-	<chem>O=S(=O)(Nc1cc(C)C)n1c1ccc(N)c2c2</chem>	0.89	0.76	-0.13	0.43	-0.46
3-pyrazolidinone, 1-phenyl-	<chem>O=C1NN(c1cccc1)c1C2C2</chem>	0.89	0.77	-0.12	0.46	-0.43
ethane, 1,1-oxybis-	<chem>O(CC)CC</chem>	0.89	1.05	0.16	1.12	0.23

2-butanol, 2-methyl-	OC(CC)(C)C	0.89	1.22	0.33	1.19	0.30
benzenamine, 4-methylbenzenesulfonate	c2ccc(cc2)N	0.90	1.08	0.18	0.89	-0.01
1,2-benzisothiazol-3(2H)-one, 1,1-dioxide	O=C(NS(=O)(=O)c1cccc2)c12	0.91	0.45	-0.46	0.09	-0.82
4,6-(1H,5H)-pyrimidinedione, 5-ethylidihydro-5-phenyl-	CCC1(C(=O)NCNC1(=O))c2ccccc2	0.91	0.73	-0.18	0.62	-0.29
2,4-pyrimidinediamine, 5-[(3,4,5-trimethoxyphenyl)methyl]-	COc2cc(Cc1cnc(N)nc1N)cc(OC)c2O	0.91	0.73	-0.18	1.26	0.35
2-pentanone	O=C(CCC)C	0.91	0.75	-0.16	0.87	-0.04
methane, chloro-	ClC	0.91	1.09	0.18	0.67	-0.24
1,4-benzenediol, 2-methyl-	Oc(c(cc(O)c1)C)c1	0.91	1.58	0.67	0.98	0.07
acetic acid, dichloro-	O=C(O)C(Cl)Cl	0.92	0.52	-0.40	0.99	0.07
ethanone, 1-(1H-pyrrol-2-yl)-	O=C(C(NC=C1)=C1)C	0.93	0.56	-0.37	0.82	-0.11
propane, 2-nitro-	N(=O)(=O)C(C)C	0.93	0.87	-0.06	0.71	-0.22
2-propenoic acid, 2-methyl-	O=C(O)C(=C)C	0.93	0.99	0.06	0.63	-0.30
propanoic acid, 2-methyl-	O=C(O)C(C)C	0.94	1.00	0.06	0.78	-0.16
1-propyne	C(#C)C	0.94	1.04	0.10	0.92	-0.02
acetic acid, chloro-, ethyl ester	O=C(OCC)CCl	0.94	1.12	0.18	1.14	0.20
methane, isothiocyanato-	N(=C=S)C	0.94	1.30	0.36	1.07	0.13
propane, 2-methoxy-2-methyl-	O(C(C)(C)C)C	0.94	1.43	0.49	1.53	0.59
1,3-dioxolo[4,5-g]quinoline-7-carboxylic acid, 5-ethyl-5,8-dihydro-8-oxo-	C1Oc2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2O1	0.94	1.70	0.76	0.86	-0.08
benzenamine, 4-methoxy-	O(c(ccc(N)c1)c1)C	0.95	1.16	0.21	1.01	0.06
2H-pyran, tetrahydro-	O(CCCC1)C1	0.95	1.43	0.48	1.16	0.21
pyrazine, trimethyl-	n(c(c(nc1C)C)C)c1	0.95	1.58	0.63	1.11	0.16
2-propenoic acid, 1,2-ethanediybis(oxy-2,1-ethanediy) ester	O=C(OCCOCCOCCOC(=O)C=C)C=C	0.96	0.57	-0.39	1.29	0.33
propanedioic acid, diethyl ester	O=C(OCC)CC(=O)OCC	0.96	0.90	-0.06	0.93	-0.03
2-propenoic acid, 2-methyl-, 2-hydroxypropyl ester	O=C(OCC(O)C)C(=C)C	0.97	0.72	-0.25	0.73	-0.24
benzenamine, 4,4-sulfonylbis-	O=S(=O)(c(ccc(N)c1)c1)c(ccc(N)c2)c2	0.97	0.77	-0.20	1.19	0.22
1-butanamine	NCCCC	0.97	0.83	-0.14	0.85	-0.12
benzenepropanenitrile, -oxo-	O=C(c(cccc1)c1)CC(#N)	0.97	0.83	-0.14	1.32	0.35
benzaldehyde, 3-hydroxy-4-methoxy-	O=Cc(ccc(OC)c1O)c1	0.97	1.05	0.08	1.36	0.39
benzeneacetic acid, alpha-(hydroxymethyl)-, (1-alpha,2-beta,4-beta,5-alpha,7-beta)-9-methyl-3-oxa-9-azatricyclo[3.3.1.0 ^{2,4}]non-7-yl ester, (-alpha)-	CN1C2CC(CCC1C3OC23)OC(=O)C(CO)c4ccccc4	0.98	0.39	-0.59	1.40	0.42
2,4,7-pteridinetriamine, 6-phenyl-	Nc3nc(N)c2nc(c1cccc1)c(N)nc2n3	0.98	0.80	-0.18	1.21	0.23
urea, N,N-dimethyl-N-phenyl-	O=C(N(C)C)Nc(cccc1)c1	0.98	1.38	0.40	1.15	0.17
strychnidin-10-one, 2,3-dimethoxy-	O=C(N(c1C1(C(N(C2)CC(C3C4C5OC6)=C6)C3)C2)cc(OC)c7OC)c7)C14)C5	0.98	1.49	0.51	1.85	0.87
3-pentanone	O=C(CC)CC	0.99	0.75	-0.24	1.19	0.20
1,1-ethanediol, 2,2,2-trichloro-	OC(O)C(Cl)(Cl)Cl	0.99	0.98	-0.01	0.88	-0.11
1,2-benzenedicarbonitrile	C(#N)c(c(C#N))ccc1c1	0.99	1.09	0.10	0.98	-0.01
2-furancarboxylic acid, methyl ester	O=C(OC)C(OC=C1)=C1	1.00	0.95	-0.05	1.21	0.21
alpha-glucofuranose, 1,2-o-(2,2,2-trichloroethylidene)-	O(C(OC(C1O)C(O)CO)C1O2)C2C(Cl)(Cl)Cl	1.02	0.68	-0.34	0.19	-0.83
2-thiophenecarboxaldehyde	O=CC(SC=C1)=C1	1.02	1.53	0.51	1.00	-0.02
hexanedioic acid, dimethyl ester	O=C(OC)CCCCC(=O)OC	1.03	1.39	0.36	0.94	-0.09
acetamide, 2,2,2-trichloro-	O=C(N)C(Cl)(Cl)Cl	1.04	0.83	-0.21	0.98	-0.06
ethene, ethoxy-	O(C=C)CC	1.04	0.91	-0.13	1.19	0.15
benzoic acid, 4-hydroxy-3,5-dimethoxy-	O=C(O)c(cc(OC)c(O)c1OC)c1	1.04	1.04	0.00	1.55	0.51
1,3-benzodioxole-5-carboxaldehyde	O=Cc(ccc(OCO1)c12)c2	1.05	1.77	0.72	0.79	-0.26
1,3-propanediol, 2,2-bis(bromomethyl)-	OC(CBr)(CBr)CO	1.06	0.85	-0.21	1.03	-0.03
pyrazine, 2-ethyl-3-methyl-	n(c(c(nc1)CC)C)c1	1.07	1.53	0.46	1.20	0.13
methane, chlorodifluoro-	FC(F)Cl	1.08	0.89	-0.19	0.98	-0.10
benzenemethanamine	NCc(cccc1)c1	1.09	1.07	-0.02	0.90	-0.19
ethanol, 2,2-[(4-methylphenyl)imino]bis-	OCCN(c(ccc1C)C)c1CCO	1.09	1.18	0.09	0.85	-0.24
benzenemethanol	OCc(cccc1)c1	1.10	1.08	-0.02	1.07	-0.03
benzenemethanol, 4-methoxy-	O(c(ccc1)CO)c1C	1.10	1.16	0.06	1.28	0.18
piperazine, 1-phenyl-	N(c(cccc1)c1)(CCNC2)C2	1.10	1.54	0.44	1.54	0.44
propanenitrile, 2,2-azobis[2-methyl-	C(#N)C(N=NC(C#N))(C)C(C)C	1.10	2.87	1.77	2.43	1.33
pyridine, 2-methyl-	n(c(ccc1)C)c1	1.11	1.35	0.24	1.25	0.14
2-propen-1-amine, N-2-propenyl-	N(CC=C)CC=C	1.11	1.52	0.41	0.87	-0.24
3,5-heptanedione	O=C(CC(=O)CC)CC	1.12	1.03	-0.09	1.18	0.06
acetic acid, bromo-, ethyl ester	O=C(OCC)CBr	1.12	1.21	0.09	1.20	0.08

benzenemethanol, 2-methoxy-	O(c(c(ccc1)CO)c1)C	1.13	1.16	0.03	1.23	0.10
ethene	C=C	1.13	1.27	0.14	0.90	-0.23
acetamide, 2,2-dichloro-N-[2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]-sulfuric acid, diethyl ester	O=C(NC(C(O)c(ccc(N(=O)=O)c1)c1)CO)C(Cl)Cl	1.14	0.92	-0.22	1.15	0.01
benzenesulfonamide, 4-chloro-2-propenoic acid, 3-(3,4-dihydroxyphenyl)-formamide, N-phenyl-	O=S(=O)(OCC)OCC	1.14	1.14	0.00	-0.29	-1.43
phenol, 2,6-dimethoxy-	O=S(=O)(N)c(ccc(c1)Cl)c1	1.15	1.01	-0.14	1.04	-0.11
2-propenal, 3-(2-furanyl)-1H-isoindeole-1,3(2H)-dione	c1c(O)c(O)ccc1C=CC(=O)O	1.15	1.11	-0.04	1.67	0.52
ethanol, 2-[2-(benzoyloxy)ethoxy]-2(3H)-benzoxazolone	O=C(Nc(cccc1)c1)C	1.15	1.13	-0.02	1.20	0.05
acetamide, N-phenyl-	O(c(c(O)c(OC)cc1)c1)C	1.15	1.16	0.01	1.29	0.14
ethanol, 2-phenoxy-	O=CC=CC(OC=C1)=C1	1.15	1.19	0.04	1.17	0.02
1,2-ethanediol, dinitrate	O=C(NC(=O)c1cccc2)c12	1.15	1.30	0.15	0.83	-0.32
1-butanol, 3-methyl-	O=C(OCCOCCO)c(cccc1)c1	1.16	0.58	-0.58	1.07	-0.09
butanoic acid, 3-methyl-	O=C(Oc(c1ccc2)c2)N1	1.16	0.95	-0.21	1.37	0.21
benzenepropanoic acid, 4-hydroxy-pyridine, 3-(1-methyl-2-pyrrolidinyl)-pyrazine, (methylthio)-	O=C(Nc(cccc1)c1)C	1.16	1.10	-0.06	1.05	-0.11
benzenamine, 2-methoxy-	O(c(cccc1)c1)CCO	1.16	1.10	-0.06	1.22	0.06
methane, tetrafluoro-	O(N(=O)=O)CCO(N(=O)=O)	1.16	1.17	0.01	1.17	0.01
butanoic acid, 2-methyl-	OCCC(C)C	1.16	1.26	0.10	1.33	0.17
benzoic acid, 2-(acetyloxy)-methane, bromo-	O=C(O)CC(C)C	1.16	1.49	0.33	1.26	0.10
pentanol	OC(=O)CCc1ccc(O)cc1	1.16	1.81	0.65	1.15	-0.01
morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, (5-alpha,6-alpha)-2H-1,2,4-benzothiadiazine, 7-chloro-3-methyl-, 1,1-dioxide	n(cccc1C(N(CC2)C)C2)c1	1.17	1.00	-0.17	0.87	-0.30
2-butanone, 3,3-dimethyl-	n1c(SC)cncc1	1.17	1.08	-0.09	0.99	-0.18
pyridine, 3-methyl-	O(c(c(N)ccc1)c1)C	1.18	1.16	-0.02	0.93	-0.25
butane, 2-nitro-	FC(F)(F)F	1.18	1.19	0.01	1.75	0.57
butanedioic acid, diethyl ester	O=C(O)C(CC)C	1.18	1.49	0.31	1.47	0.29
ethane, 1,1,1-[methylidynetris(oxy)]tris-	O=C(Oc(c(ccc1)C(=O)O)c1)C	1.19	1.13	-0.06	1.43	0.24
benzaldehyde, 4-hydroxy-3-methoxy-carbonic acid, diethyl ester	BrC	1.19	1.18	-0.01	0.68	-0.51
3-pentanol	CC(CCC)O	1.19	1.26	0.07	1.18	-0.01
benzoic acid, 2-amino-	COc1ccc2CC5C3C=CC(O)C4Oc1c2	1.19	1.28	0.09	1.20	0.01
propanoic acid, ethyl ester	C34CCN5C					
1H-pyrrole, 1-methyl-	Clc1ccc2N=C(C)NS(=O)(=O)c2c1	1.20	1.01	-0.19	0.96	-0.24
pyridine, 4-methyl-	O=C(C(C)(C)C)C	1.20	1.13	-0.07	1.59	0.39
benzaldehyde, 3,4-dimethoxy-cyclohexanol	n(cccc1C)c1	1.20	1.35	0.15	1.11	-0.09
ethene, 1,1-difluoro-	CCC(N(=O)=O)C	1.20	1.36	0.16	1.49	0.29
2,4-pyrimidinediamine, 6-(1-piperidinyl)-, 3-oxide	O=C(OCC)CCC(=O)OCC	1.20	1.39	0.19	1.25	0.05
acetic acid, propyl ester	O(C(OCC)OCC)CC	1.20	1.45	0.25	0.99	-0.21
furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-6(5aH)-one, 5,8,8a,9-tetrahydro-5-(4-hydroxy-3,5-dimethoxyphenyl)-9-[[4,6-o-[2-thienylmethylene]-beta-glucopyranosyl]oxy]-	O=Cc(ccc(O)c1OC)c1	1.21	1.05	-0.16	1.31	0.10
pyrazine, 2-methoxy-3-methyl-	O=C(OCC)OCC	1.21	1.22	0.01	0.86	-0.35
1,3-pentanediol, 2,2,4-trimethyl-	OC(CC)CC	1.21	1.26	0.05	1.22	0.01
benzenamine, 4-ethoxy-	O=C(O)c(c(N)ccc1)c1	1.21	1.36	0.15	0.78	-0.43
ethanedione, di-2-furanyl-	O=C(OCC)CC	1.21	1.36	0.15	1.32	0.11
hydrazine, phenyl-	C1=CN(C)C=C1	1.21	1.43	0.22	1.31	0.10
methane, dichloro-	n(ccc(c1)C)c1	1.22	1.35	0.13	1.14	-0.08
2-propenoic acid, oxybis(2,1-ethanediyl)-2,1-ethanediyl ester	O=Cc(ccc(OC)c1OC)c1	1.22	1.36	0.14	1.64	0.42
2(1H)-quinolinone	OC(CCCC1)C1	1.23	1.64	0.41	1.35	0.12
5,12-naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-alpha-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-	FC(F)=C	1.24	1.24	0.00	1.56	0.32
benzamide, 2-hydroxy-	C1CCCCN1c2nc(N(=O)c(N)c2	1.24	1.35	0.11	1.24	0.00
2,5-cyclohexadiene, 1,4-dione, 2,5-dimethyl-	O=C(OCCC)C	1.24	1.36	0.12	1.28	0.04
	COc1cc(cc(OC)c1OC)C2C3C(COC3=O)C(OC4OC5COC(OC5C(O)C4O)c6cccs6)c7cc8OCOC8cc27	1.24	1.42	0.18	1.97	0.73
	O(c(ncn1)c1C)C	1.24	1.46	0.22	1.09	-0.15
	OCC(C(O)C(C)C)(C)C	1.24	1.49	0.25	1.08	-0.16
	O(c(ccc(N)c1)c1)CC	1.24	1.65	0.41	1.64	0.40
	o1cccc1C(=O)C(=O)c2occc2	1.24	1.80	0.56	1.55	0.31
	N(N)c(cccc1)c1	1.25	0.79	-0.46	0.95	-0.30
	CICCl	1.25	1.34	0.09	1.12	-0.13
	O=C(OCCOCCOCCOCCOC(=O)C=C)C=C	1.26	0.29	-0.97	1.10	-0.16
	c1ccc2C=CC(=O)Nc2c1	1.26	1.32	0.06	1.51	0.25
	COc4cccc5C(=O)c3c(O)c2CC(O)(CC(OC1CC(N)C(O)C(C)O1)c2c(O)c3C(=O)c45)C(=O)CO	1.27	1.85	0.58	1.41	0.14
	O=C(N)c(c(O)ccc1)c1	1.28	1.03	-0.25	0.74	-0.54
	O=C1C(C)=CC(=O)C(C)=C1	1.28	1.34	0.06	1.11	-0.17

4,4-bipyridine	<chem>n(ccc(c1)c(ccnc2)c2)c1</chem>	1.28	1.38	0.10	1.40	0.12
pyrazine, tetramethyl-	<chem>n(c(c(nc1C)C)C)c1C</chem>	1.28	2.13	0.85	1.46	0.18
1-butanol, 2-methyl-	<chem>OCC(CC)C</chem>	1.29	1.26	-0.03	1.24	-0.05
butanoic acid, methyl ester	<chem>O=C(OC)CCC</chem>	1.29	1.36	0.07	1.22	-0.07
acetamide, N-(5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo[a]heptalen-7-yl)-	<chem>O=C(NC(C(C(c(cc(OC)c1OC)C2)c1OC)=CC=C(OC)C3(=O))=C3)C2)C</chem>	1.30	1.86	0.56	1.59	0.29
glucitol, 1,4:3,6-dianhydro-, dinitrate	<chem>O(N(=O)=O)C(C(OCC1O(N(=O)=O))C1O2)C2</chem>	1.31	0.76	-0.55	0.87	-0.44
2-pentanone, 4-methyl-	<chem>O=C(CC(C)C)C</chem>	1.31	1.16	-0.15	1.31	0.00
quinoxaline	<chem>n(c(c(nc1)ccc2)c2)c1</chem>	1.32	1.12	-0.20	1.12	-0.20
3-pyridinecarboxylic acid, ethyl ester	<chem>O=C(OCC)c(cccn1)c1</chem>	1.32	1.13	-0.19	1.17	-0.15
2-propenoic acid, ethyl ester	<chem>O=C(OCC)C=C</chem>	1.32	1.22	-0.10	1.24	-0.08
phenol, 2-methoxy-	<chem>O(c(c(O)ccc1)c1)C</chem>	1.32	1.34	0.02	1.32	0.00
benzenamine, 2-methyl-	<chem>Nc(c(ccc1)C)c1</chem>	1.32	1.62	0.30	1.32	0.00
acetic acid, trichloro-	<chem>O=C(O)C(Cl)(Cl)Cl</chem>	1.33	1.44	0.11	1.17	-0.16
phenol, 2,4,6-trinitro-	<chem>N(=O)(=O)c(cc(N(=O)=O)(=O))c(O)c1N(=O)(=O)c1</chem>	1.33	1.54	0.21	1.83	0.50
2,4-hexadienoic acid, (E,E)-	<chem>O=C(O)C=CC=CC</chem>	1.33	1.62	0.29	1.77	0.44
4-pyridinamine, N,N-dimethyl-	<chem>n(ccc(N(C)C)C)c1</chem>	1.34	0.98	-0.36	1.36	0.02
acetic acid, phenoxy-	<chem>O=C(O)COc(cccc1)c1</chem>	1.34	1.33	-0.01	1.48	0.14
furan	<chem>O1C=CC=C1</chem>	1.34	1.36	0.02	1.24	-0.10
1,4-naphthalenedione, 2-methoxy-	<chem>c1ccc2C(=O)C=C(OC)C(=O)c2c1</chem>	1.35	0.95	-0.40	1.70	0.35
benzaldehyde, 4-hydroxy-	<chem>O=Cc(ccc(O)c1)c1</chem>	1.35	1.23	-0.12	1.27	-0.08
3-buten-2-one, 4-(2-furanyl)-	<chem>O=C(C=CC(OC=C1)=C1)C</chem>	1.35	1.41	0.06	1.42	0.07
4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[aminophenylacetyl]amino]-3,3-dimethyl-7-oxo	<chem>CC3(C)SC2C(NC(=O)C(N)c1ccccc1)C(=O)N2C3C(=O)(O)</chem>	1.35	1.45	0.10	0.88	-0.47
benzeneethanol	<chem>OCCc(cccc1)c1</chem>	1.36	1.57	0.21	1.51	0.15
benzenamine, 3-nitro-	<chem>N(=O)(=O)c(cccc1N)c1</chem>	1.37	1.47	0.10	1.53	0.16
benzaldehyde, 2-hydroxy-3-methoxy-	<chem>O=Cc(c(O)c(OC)cc1)c1</chem>	1.37	1.83	0.46	1.31	-0.06
2-hexanone	<chem>O=C(CCCC)C</chem>	1.38	1.24	-0.14	1.45	0.07
2-propenoic acid, 2-methyl-, methyl ester	<chem>O=C(OC)C(=C)C</chem>	1.38	1.28	-0.10	1.10	-0.28
cyclohexanone, 4-methyl-	<chem>O=C(CCC(C1)C)C1</chem>	1.38	1.54	0.16	1.46	0.08
phenol, 2-methoxy-, acetate	<chem>COc1ccccc1OC(=O)C</chem>	1.38	1.67	0.29	1.64	0.26
pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-	<chem>N=C(N(CCCC1CC2)C1)C2</chem>	1.38	2.70	1.32	1.60	0.22
1,2-propanediol, 3-(2-methoxyphenoxy)-	<chem>O(c(c(OC)ccc1)c1)CC(O)CO</chem>	1.39	0.42	-0.97	0.76	-0.63
benzenamine, 4-nitro-	<chem>N(=O)(=O)c(ccc(N)c1)c1</chem>	1.39	1.47	0.08	1.50	0.11
2H-1-benzopyran-2-one	<chem>c1cc2OC(=O)C=Cc2cc1</chem>	1.39	1.51	0.12	1.72	0.33
pentanoic acid	<chem>O=C(O)CCCC</chem>	1.39	1.56	0.17	1.34	-0.05
benzenamine, 4-methyl-	<chem>Cc1ccc(N)cc1</chem>	1.39	1.62	0.23	1.34	-0.05
2H-1,3,5-thiadiazine-2-thione, tetrahydro-3,5-dimethyl-	<chem>N(CSC(N1C)=S)(C1)C</chem>	1.40	0.94	-0.46	0.48	-0.92
carbamic acid, [1,2-phenylenebis(iminocarbonothioyl)]bis-, dimethyl ester	<chem>COC(=O)NC(=S)Nc1ccccc1NC(=S)N</chem>	1.40	1.10	-0.30	1.57	0.17
benzonitrile, 2-amino-	<chem>N#Cc(c(N)ccc1)c1</chem>	1.40	1.17	-0.23	1.05	-0.35
benzenamine, 3-methyl-	<chem>Nc(cccc1C)c1</chem>	1.40	1.62	0.22	1.32	-0.08
2-propanamine, N-(1-methylethyl)-	<chem>N(C(C)C)C(C)C</chem>	1.40	1.64	0.24	1.12	-0.28
1,4-benzenediol, 2-chloro-	<chem>Oc(c(cc(O)c1)Cl)c1</chem>	1.40	1.68	0.28	1.62	0.22
hydrazine, (4-nitrophenyl)-	<chem>N(=O)(=O)c(ccc(NN)c1)c1</chem>	1.41	1.19	-0.22	1.27	-0.14
benzeneethanamine	<chem>NCCc(cccc1)c1</chem>	1.41	1.34	-0.07	1.41	0.00
methane, bromochloro-	<chem>BrCCl</chem>	1.41	1.43	0.02	1.27	-0.14
benzeneacetic acid	<chem>O=C(O)Cc(cccc1)c1</chem>	1.41	1.43	0.02	1.72	0.31
1H-indole-3-acetic acid	<chem>O=C(O)CC(c(c(N1)ccc2)c2)=C1</chem>	1.41	1.49	0.08	1.87	0.46
acetic acid, phenoxy-, methyl ester	<chem>O=C(OC)COc(cccc1)c1</chem>	1.41	1.61	0.20	1.90	0.49
benzenemethanol, alpha-methyl-	<chem>OC(c(cccc1)c1)C</chem>	1.42	1.49	0.07	1.58	0.16
benzeneacetic acid, 4-methoxy-	<chem>O=C(O)Cc(ccc(OC)c1)c1</chem>	1.42	1.51	0.09	1.73	0.31
ethane, chloro-	<chem>ClCC</chem>	1.43	1.58	0.15	1.47	0.04
benzenethiol, 2-amino-	<chem>Sc(c(N)ccc1)c1</chem>	1.43	1.77	0.34	1.52	0.09
1H-benzotriazole	<chem>c1ccc2nnnc2c1</chem>	1.44	1.17	-0.27	1.19	-0.25
ethanone, 1-(methylphenyl)-	<chem>c(ccc1CC(=O)C)cc1</chem>	1.44	1.47	0.03	1.70	0.26
ethanol, 2-chloro-, phosphate (3:1)	<chem>O=P(OCCCl)(OCCCl)OCCCl</chem>	1.44	1.63	0.19	1.36	-0.08
ethanamine, N,N-diethyl-	<chem>N(CC)(CC)CC</chem>	1.45	1.51	0.06	1.57	0.12
1,2-propadiene	<chem>C=C=C</chem>	1.45	1.65	0.20	1.67	0.22
1,3-butanedione, 4,4,4-trifluoro-1-(2-thienyl)-	<chem>O=C(C(SC=C1)=C1)CC(=O)C(F)(F)F</chem>	1.46	0.84	-0.62	2.37	0.91
benzoic acid, 2-nitro-	<chem>O=C(O)c(c(N(=O)=O))ccc1)c1</chem>	1.46	1.35	-0.11	1.50	0.04
phenol	<chem>Oc(cccc1)c1</chem>	1.46	1.51	0.05	1.39	-0.07
2-butyne	<chem>C(#CC)C</chem>	1.46	1.59	0.13	1.70	0.24

benzene, 1,4-dinitro-	<chem>N(=O)(=O)c(ccc(N(=O)=O))c1c1</chem>	1.46	1.63	0.17	1.70	0.24
phosphoric acid, 2,2-dichloroethenyl dimethyl ester	<chem>O=P(OC)(OC)OC=C(Cl)Cl</chem>	1.47	0.60	-0.87	1.27	-0.20
hydrazine, (2,4-dinitrophenyl)-	<chem>N(=O)(=O)c(ccc(NN)c1N(=O)=O))c1</chem>	1.47	1.01	-0.46	1.27	-0.20
2,4,6-(1H,3H,5H)-pyrimidinetrione, 5-ethyl-5-phenyl-	<chem>CCC1(C(=O)NC(=O)NC1(=O))c2ccc</chem>	1.47	1.33	-0.14	1.40	-0.07
	<chem>cc2</chem>					
benzaldehyde, 3-nitro-	<chem>O=Cc(cccc1N(=O)=O))c1</chem>	1.47	1.53	0.06	1.48	0.01
propanoic acid, 2,2-dimethyl-	<chem>O=C(O)C(C)(C)C</chem>	1.48	1.45	-0.03	1.37	-0.11
benzaldehyde	<chem>O=Cc(cccc1)c1</chem>	1.48	1.71	0.23	1.60	0.12
ethane, 1,2-dichloro-	<chem>ClCCCl</chem>	1.48	1.83	0.35	1.48	0.00
1-pentanamine	<chem>NCCCCC</chem>	1.49	1.33	-0.16	1.39	-0.10
acetic acid, phenyl ester	<chem>O=C(OC(c(cccc1)c1)C</chem>	1.49	1.59	0.10	1.59	0.10
cyclohexanamine	<chem>NC(CCCCC1)C1</chem>	1.49	1.63	0.14	1.30	-0.19
benzene, 1,3-dinitro-	<chem>N(=O)(=O)c(cccc1N(=O)=O))c1</chem>	1.49	1.63	0.14	1.70	0.21
2,5-cyclohexadiene-1,4-dione, dioxime	<chem>ON=C1C=CC(=NO)C=C1</chem>	1.49	1.92	0.43	0.03	-1.46
1H-benzimidazole, 5-nitro-	<chem>N(=O)(=O)c(ccc(ncn1)c12)c2</chem>	1.50	1.05	-0.45	1.77	0.27
2,2-bipyridine	<chem>n(c(ccc1)c(nccc2)c2)c1</chem>	1.50	1.38	-0.12	1.85	0.35
benzeneacetic acid, 3-methoxy-	<chem>OC(=O)Cc1cc(OC)ccc1</chem>	1.50	1.51	0.01	1.71	0.21
1-pentanol	<chem>CCCCC</chem>	1.51	1.33	-0.18	1.47	-0.04
methane, iodo-	<chem>Cl</chem>	1.51	1.59	0.08	1.20	-0.31
pyrazine, 2,3-diethyl-	<chem>n(c(c(nc1)CC)CC)c1</chem>	1.51	2.02	0.51	1.73	0.22
bicyclo[2.2.1]heptane-2,3-dione, 1,7,7-trimethyl-	<chem>CC1(C)C2CCC1(C)C(=O)C2(=O)</chem>	1.52	0.75	-0.77	2.57	1.05
carbamic acid, 1H-benzimidazol-2-yl-, methyl ester	<chem>c1ccc2nc(NC(=O)OC)nc2c1</chem>	1.52	1.55	0.03	0.99	-0.53
propane, 2,2-oxybis-	<chem>O(C(C)C)C(C)C</chem>	1.52	1.88	0.36	1.69	0.17
phenol, 2-(1-methylethoxy)-, methylcarbamate	<chem>CNC(=O)Oc1cccc1OC(C)C</chem>	1.52	1.90	0.38	1.97	0.45
urea, N,N'-bis(2-chloroethyl)-N-nitroso-	<chem>ClCCNC(=O)N(CCCl)N=O</chem>	1.53	1.44	-0.09	1.24	-0.29
benzene, 1,2,3-trimethoxy-	<chem>O(c(c(OC)ccc1)c1OC)C</chem>	1.53	1.50	-0.03	2.02	0.49
phenol, 2-amino-6-chloro-4-nitro-	<chem>N(=O)(=O)c(cc(N)c(O)c1Cl)c1</chem>	1.53	1.64	0.11	1.96	0.43
2,3-naphthalenediamine	<chem>c(c(ccc1)cc(N)c2N)(c1)c2</chem>	1.54	1.34	-0.20	1.41	-0.13
ethane, (methylthio)-	<chem>S(CC)C</chem>	1.54	1.41	-0.13	1.16	-0.38
4H-1-benzopyran-4-one, 2-(2,4-dihydroxyphenyl)-	<chem>Oc1cc(O)c2C(=O)C(O)=C(c3ccc(O)c</chem>	1.54	1.48	-0.06	2.23	0.69
	<chem>c3O)Oc2c1</chem>					
pyridine, 2-ethenyl-	<chem>n(c(ccc1)C=C)c1</chem>	1.54	1.71	0.17	1.48	-0.06
methane, dichlorofluoro-	<chem>FC(Cl)Cl</chem>	1.55	1.21	-0.34	1.28	-0.27
benzoic acid, 3,5-dinitro-	<chem>O=C(O)c(cc(N(=O)=O))cc1N(=O)</chem>	1.55	1.51	-0.04	1.64	0.09
	<chem>(=O))c1</chem>					
benzeneacetic acid, 4-fluoro-	<chem>O=C(O)Cc(ccc(F)c1)c1</chem>	1.55	1.63	0.08	1.79	0.24
1,3-benzenediol, 2-nitro-	<chem>N(=O)(=O)c(c(O)ccc1)c1O</chem>	1.56	1.43	-0.13	1.29	-0.27
benzaldehyde, 4-nitro-	<chem>O=Cc(ccc(N(=O)=O))c1c1</chem>	1.56	1.53	-0.03	1.45	-0.11
benzonitrile	<chem>C(#N)c(cccc1)c1</chem>	1.56	1.54	-0.02	1.55	-0.01
benzeneacetonitrile	<chem>C(#N)Cc(cccc1)c1</chem>	1.56	1.56	0.00	1.42	-0.14
1H-purin-6-amine, N-(phenylmethyl)-	<chem>n(c(NC(c(cccc1)c1)c(N=CN2)c2n3)c3</chem>	1.57	1.23	-0.34	1.79	0.22
	<chem>BrC=C</chem>	1.57	1.52	-0.05	1.19	-0.38
ethene, bromo-	<chem>O=C(O)CCCCCCCC(=O)O</chem>	1.57	1.70	0.13	1.37	-0.20
nonanedioic acid	<chem>n(c(c(nc1)CCC)C)c1</chem>	1.57	2.02	0.45	1.64	0.07
pyrazine, 2-methyl-3-propyl-	<chem>Oc1ccc2C=CC(=O)Oc2c1</chem>	1.58	1.03	-0.55	1.85	0.27
2H-1-benzopyran-2-one, 7-hydroxy-	<chem>O=C(O)c(ccc(O)c1)c1</chem>	1.58	1.39	-0.19	1.58	0.00
benzoic acid, 4-hydroxy-	<chem>O=Cc(ccc(O)c1OCC)c1</chem>	1.58	1.55	-0.03	1.82	0.24
benzaldehyde, 3-ethoxy-4-hydroxy-	<chem>O(c(ccc(O)c1)c1)C</chem>	1.58	1.59	0.01	1.31	-0.27
phenol, 4-methoxy-	<chem>OCc(ccc(c1)C)c1</chem>	1.58	1.62	0.04	1.54	-0.04
benzenemethanol, 4-methyl-	<chem>CC(=O)Nc1ccc(OCC)cc1</chem>	1.58	1.67	0.09	1.62	0.04
acetamide, N-(4-ethoxyphenyl)-	<chem>O=C(c(c(cccc1)c1)C</chem>	1.58	1.67	0.09	1.65	0.07
ethanone, 1-phenyl-	<chem>O=C(O)c(c(OC)ccc1)c1</chem>	1.59	1.61	0.02	1.67	0.08
benzoic acid, 2-methoxy-	<chem>Cc1ccc2C(=O)C(C(=O)O)=CN(CC)c</chem>	1.59	1.64	0.05	0.95	-0.64
	<chem>2n1</chem>					
1,8-naphthyridine-3-carboxylic acid, 1-ethyl-1,4-	<chem>N1C(=Nc2c(Cl)cccc2Cl)NCC1</chem>	1.59	1.89	0.30	1.92	0.33
dihydro-7-methyl-4-oxo-						
1H-imidazol-2-amine, N-(2,6-dichlorophenyl)-4,5-						
dihydro-	<chem>Nc(ccc(c1)Cc(ccc(N)c2)c2)c1</chem>	1.59	2.18	0.59	2.04	0.45
benzenamine, 4,4-methylenebis-	<chem>C(#N)c(ccc(O)c1)c1</chem>	1.60	1.61	0.01	1.68	0.08
benzonitrile, 4-hydroxy-	<chem>O(c(c(OC)ccc1)c1)C</chem>	1.60	1.64	0.04	2.10	0.50
benzene, 1,2-dimethoxy-	<chem>O=C(OC)c(c(ccc1)C(=O)OC)c1</chem>	1.60	1.66	0.06	1.96	0.36
1,2-benzenedicarboxylic acid, dimethyl ester	<chem>N(=O)(=O)c(cc(N(=O)</chem>	1.60	1.99	0.39	1.50	-0.10
benzene, 2-methyl-1,3,5-trinitro-	<chem>(=O))c(c1N(=O)=O))C)c1</chem>					
	<chem>O=C(OC(=O)c1cccc2)c12</chem>	1.60	2.07	0.47	0.89	-0.71
1,3-isobenzofurandione	<chem>O=C(O)c(ccc(OC)c1OC)c1</chem>	1.61	1.52	-0.09	1.52	-0.09
benzoic acid, 3,4-dimethoxy-	<chem>O(c(cccc1)c1)CC(O)C</chem>	1.61	1.52	-0.09	1.70	0.09
2-propanol, 1-phenoxy-	<chem>O(C1c(cccc2)c2)C1</chem>	1.61	1.59	-0.02	1.72	0.11
oxirane, phenyl-	<chem>O=C(C(O)</chem>	1.61	1.62	0.01	1.79	0.18
pregn-4-ene-3,20-dione, 11,17,21-trihydroxy-, (11)-						

	(C/C(C(C(C(C(=CC(=O)C1)C2) (C1)C)C3O)C2)C4)(C3)C)C4)CO					
ethane, bromo-	BrCC	1.61	1.67	0.06	1.64	0.03
pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-, (11)-	C1C2=CC(=O)C=CC2(C)C3C(O)CC 4(C)C(O)(C(=O)CO)CCC4C3C1	1.62	1.40	-0.22	1.66	0.04
1,2,3-propanetriol, trinitrate	O(N(=O)=O)CC(O(N(=O)=O))CO(N(=O)=O)	1.62	1.51	-0.11	1.25	-0.37
3-quinolinamine	n(c(c(ccc1)cc2N)c1)c2	1.63	1.23	-0.40	1.57	-0.06
ethanone, 1-(2-aminophenyl)-	O=C(c(c(N)ccc1)c1)C	1.63	1.57	-0.06	0.98	-0.65
benzaldehyde, 4-ethoxy-3-methoxy-	O=Cc(ccc(OC)c1OC)c1	1.63	1.85	0.22	2.18	0.55
1H-tetrazole, 5-phenyl-	N1N=NN=C1c2ccccc2	1.65	0.18	-1.47	1.14	-0.51
methane, chlorotrifluoro-	CC(F)(F)Cl	1.65	1.50	-0.15	1.80	0.15
2,4,6-(1H,3H,5H)-pyrimidinetrione, 5-ethyl-5-(1- methylpropyl)-	CCC(C)C1(CC)C(=O)NC(=O)NC1(=O)	1.65	1.51	-0.14	1.70	0.05
benzoic acid, 2-(acetylmino)-, methyl ester	O=C(Nc(c(ccc1)C(=O)OC)c1)C	1.65	1.73	0.08	1.46	-0.19
3-hexanol	OC(CCC)CC	1.65	1.75	0.10	1.76	0.11
2-propanol, 1,1,1,3,3,3-hexafluoro-	FC(F)(F)C(O)C(F)(F)F	1.66	1.11	-0.55	2.58	0.92
benzenamine, N-methyl-	N(c(cccc1)c1)C	1.66	1.62	-0.04	1.68	0.02
acetamide, N-(4-nitrophenyl)-	O=C(Nc(ccc(N(=O))(=O))c1)c1)C	1.66	1.64	-0.02	1.19	-0.47
benzoic acid, 2-nitro-, methyl ester	O=C(OC)c(c(N(=O))(=O))ccc1)c1	1.66	1.65	-0.01	1.71	0.05
1,3-benzenedicarboxylic acid	O=C(O)c(cccc1C(=O)O)c1	1.66	1.76	0.10	1.04	-0.62
pyridine, 3-ethyl-	n(cccc1CC)c1	1.66	1.84	0.18	1.63	-0.03
2h-benzimidazole-2-thione, 1,3-dihydro-	N(c(c(N1)ccc2)c2)=C1S	1.66	1.93	0.27	2.20	0.54
phenol, 2,4-dinitro-	N(=O)(=O)c(ccc(O)c1N(=O)(=O))c1	1.67	1.73	0.06	1.89	0.22
1-propanamine, N-propyl-	N(CCC)CCC	1.67	1.79	0.12	1.74	0.07
pyridine, 2,6-dimethyl-	n(c(ccc1)C)c1C	1.68	1.90	0.22	1.60	-0.08
butanoic acid, 2-ethyl-	O=C(O)C(CC)CC	1.68	1.98	0.30	1.74	0.06
ethanol, 2-[2-(hexyloxy)ethoxy]-	O(CCOCCO)CCCCC	1.70	1.27	-0.43	1.65	-0.05
methane, dibromo-	BrCBr	1.70	1.52	-0.18	1.48	-0.22
acetamide, N-(4-methylphenyl)-	O=C(Nc(ccc(c1)C)c1)C	1.70	1.65	-0.05	1.28	-0.42
1,3-benzodioxol-4-ol, 2,2-dimethyl-, methylcarbamate	CNC(=O)Oc1cccc2OC(C)(C)Oc12	1.70	2.55	0.85	1.53	-0.17
2-cyclohexen-1-one, 3,5,5-trimethyl-	O=C(C=C(CC1(C)C)C)C1	1.70	2.62	0.92	1.90	0.20
butanamide, N-[3-acetyl-4-[2-hydroxy-3-[(1- methylethyl)amino]propoxy]phenyl]-	CC(=O)c1cc(NC(=O)CCC)ccc1OCC(O)CNC(C)C	1.71	1.19	-0.52	1.43	-0.28
1,4-naphthalenedione	c1cc2C(=O)C=CC(=O)c2cc1	1.71	1.66	-0.05	1.61	-0.10
benzaldehyde, 3-methoxy-	O=Cc(cccc1OC)c1	1.71	1.79	0.08	1.62	-0.09
benzoic acid, 2-hydroxy-3,5-dinitro-	O=C(O)c(c(O)c(N(=O))(=O))cc1N(=O)(=O)c1	1.71	2.46	0.75	1.80	0.09
cyclopropane	C(C1)C1	1.72	1.70	-0.02	1.56	-0.16
acetic acid, 1-methylpropyl ester	O=C(OC(CC)C)C	1.72	1.77	0.05	1.97	0.25
benzaldehyde, 2-methoxy-	O=Cc(c(OC)ccc1)c1	1.72	1.79	0.07	1.59	-0.13
ethanone, 1-(4-fluorophenyl)-	O=C(c(ccc(F)c1)c1)C	1.72	1.87	0.15	1.80	0.08
thioperoxydicarbonic diamide, tetramethyl-	N(C(=S)SSC(N(C)C)=S)(C)C	1.73	1.70	-0.03	2.18	0.45
cyclohexanol, 1-ethynyl-	OC(C#C)(CCCC1)C1	1.73	1.81	0.08	1.09	-0.64
benzaldehyde, 2-nitro-	O=Cc(c(N(=O))(=O))ccc1)c1	1.74	1.53	-0.21	1.36	-0.38
2H-1-benzopyran-2-one, 7-methoxy-	OCc1ccc2C=CC(=O)Oc2c1	1.74	1.59	-0.15	1.88	0.14
ethanone, 1-(4-methoxyphenyl)-	O=C(c(ccc(OC)c1)c1)C	1.74	1.75	0.01	1.82	0.08
benzoic acid, 2,5-dihydroxy-	O=C(O)c(c(O)ccc1O)c1	1.74	1.76	0.02	1.23	-0.51
benzenamine, 2-ethyl-	Nc(c(ccc1)CC)c1	1.74	2.11	0.37	1.91	0.17
2-propanol, 1-(1H-indol-4-yloxy)-3-[(1- methylethyl)amino]-	c12ccnc1cccc2OCC(O)CNC(C)C	1.75	1.48	-0.27	2.17	0.42
butanamide, N,N'-(3,3'-dimethyl[1,1'-biphenyl]-4,4'- diyl)bis[3-oxo-]	O=C(Nc(c(ccc1)cc(NC(=O)CC(=O)C)c1)C)c2)CC(=O)C	1.75	1.75	0.00	2.50	0.75
piperidine, 1-ethyl-	N(CCCC1)(C1)CC	1.75	1.89	0.14	2.11	0.36
acetic acid, 1,1-dimethylethyl ester	O=C(OC(C)(C)C)C	1.76	1.74	-0.02	1.88	0.12
2-hexanol	OC(CCCC)C	1.76	1.75	-0.01	1.75	-0.01
benzeneethanamine, alpha-methyl-	NC(C)Cc(cccc1)c1	1.76	1.76	0.00	1.85	0.09
benzaldehyde, 4-methoxy-	O=Cc(ccc(OC)c1)c1	1.76	1.79	0.03	1.64	-0.12
2(3H)-benzothiazolone	O=C(Nc(c1ccc2)c2)S1	1.76	2.35	0.59	1.31	-0.45
1-propene	C(=C)C	1.77	1.68	-0.09	1.68	-0.09
disulfide, dimethyl	S(SC)C	1.77	1.87	0.10	1.15	-0.62
1,8-naphthalenediamine	c(c(c(N)cc1)c(N)cc2)(c1)c2	1.78	1.34	-0.44	1.22	-0.56
benzeneacetaldehyde	O=CCc(cccc1)c1	1.78	1.54	-0.24	1.75	-0.03
acetic acid, 2-methylpropyl ester	O=C(OC(C)C)C	1.78	1.77	-0.01	1.74	-0.04
hexanal	O=CCCCC	1.78	1.80	0.02	2.37	0.59
acetic acid, butyl ester	O=C(OCCCC)C	1.78	1.85	0.07	1.84	0.06

1,10-phenanthroline	<chem>n(c(c(ccc1ccc2)cc3)c12)c3</chem>	1.78	2.29	0.51	2.31	0.53
ethane, 1,1-dichloro-	<chem>C(Cl)(Cl)C</chem>	1.79	1.76	-0.03	1.72	-0.07
phenol, 2-nitro-	<chem>N(=O)(=O)c(c(O)ccc1)c1</chem>	1.79	1.91	0.12	1.91	0.12
1-propene, 3-bromo-	<chem>BrCC=C</chem>	1.79	2.02	0.23	1.98	0.19
8-quinolinamine	<chem>n(c(c(ccc1)cc2)c1N)c2</chem>	1.79	2.03	0.24	1.51	-0.28
1,3-benzenediol, 4-chloro-	<chem>Oc(c(ccc1O)Cl)c1</chem>	1.80	1.68	-0.12	1.54	-0.26
benzoic acid, 3,4,5-trihydroxy-, propyl ester	<chem>O=C(OCCC)c(cc(O)c(O)c1O)c1</chem>	1.80	1.79	-0.01	1.84	0.04
pyrazine, 2-ethyl-3-methoxy-	<chem>O(c(nccn1)c1CC)C</chem>	1.80	1.95	0.15	1.64	-0.16
pentanoic acid, 2-methyl-	<chem>O=C(O)C(CCC)C</chem>	1.80	1.98	0.18	1.79	-0.01
ethane	<chem>CC</chem>	1.81	1.32	-0.49	1.44	-0.37
pyrazine, 2-methyl-3-(methylthio)-	<chem>n(c(SC)c(nc1)C)c1</chem>	1.81	1.63	-0.18	1.42	-0.39
1-propanethiol	<chem>SCCC</chem>	1.81	1.76	-0.05	1.72	-0.09
thiophene	<chem>S1C=CC=C1</chem>	1.81	1.81	0.00	1.89	0.08
benzaldehyde, 4-(dimethylamino)-	<chem>O=Cc(ccc(N(C)C)c1)c1</chem>	1.81	1.89	0.08	1.80	-0.01
benzenesulfonic acid, 4-methyl-, ethyl ester	<chem>O=S(=O)(OCC)c(ccc(c1)C)c1</chem>	1.81	1.96	0.15	1.77	-0.04
benzaldehyde, 2-hydroxy-	<chem>O=C(c(O)ccc1)c1</chem>	1.81	2.01	0.20	1.22	-0.59
phenol, 4-ethoxy-	<chem>O(c(ccc(O)c1)CC)</chem>	1.81	2.08	0.27	1.92	0.11
[1,1'-biphenyl]-4,4'-diamine, 3,3'-dimethoxy-	<chem>O(c(c(N)ccc1c(ccc(N)c2OC)c2)c1)C</chem>	1.81	2.08	0.27	2.02	0.21
ethanone, 1-(2-methoxyphenyl)-	<chem>O=C(c(c(OC)ccc1)c1)C</chem>	1.82	1.75	-0.07	1.71	-0.11
pyrazine, 2-ethoxy-3-methyl-	<chem>O(c(nccn1)c1C)CC</chem>	1.82	1.95	0.13	1.64	-0.18
3,6-acridinediamine	<chem>n(c(c(ccc1N)cc2ccc(N)c3)c1)c23</chem>	1.83	1.48	-0.35	2.10	0.27
benzoic acid, 3-nitro-	<chem>O=C(O)c(cccc1N(=O)(=O))c1</chem>	1.83	1.69	-0.14	1.52	-0.31
benzenamine, 4-chloro-	<chem>Nc(ccc(c1)Cl)c1</chem>	1.83	1.72	-0.11	1.95	0.12
2-propanol, 1-[(1,1-dimethylethyl)amino]-3-[[4-(4-morpholinyl)-1,2,5-thiadiazol-3-yl]oxy]-, 2-butenedioate (1:1)	<chem>N1(C2=NSN=C2OCC(O)CNC(C)(C)C)CCOCC1</chem>	1.83	1.75	-0.08	1.44	-0.39
4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-7-oxo-6-[(phenylacetyl)amino]-	<chem>O=C(NC(C(=O)N1C(C(=O)O)C(S2)(C)C)C12)Cc(cccc3)c3</chem>	1.83	1.85	0.02	1.92	0.09
benzeneacetic acid, methyl ester	<chem>O=C(OC)Cc(cccc1)c1</chem>	1.83	2.08	0.25	2.03	0.20
5,12-naphthacenedione, 8-acetyl-10-[(3-amino-2,3,6-trideoxy-alpha-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-1-methoxy-	<chem>COc4cccc5C(=O)c3c(O)c2CC(O)(CC(OC1CC(N)C(O)C(C)O1)c2c(O)c3C(=O)c45)C(C)=O</chem>	1.83	2.19	0.36	1.68	-0.15
cyclohexanol, 2-methyl-	<chem>OC(C(CCC1)C)C1</chem>	1.84	2.05	0.21	1.80	-0.04
benzenamine, 2,6-dimethyl-	<chem>Nc(c(ccc1)C)c1C</chem>	1.84	2.17	0.33	1.77	-0.07
benzenepropanoic acid	<chem>O=C(O)CCc(cccc1)c1</chem>	1.84	2.29	0.45	1.84	0.00
imidazo[2,1-b]thiazole, 2,3,5,6-tetrahydro-6-phenyl-	<chem>N3=C2N(CC3c1ccccc1)CCS2</chem>	1.84	2.87	1.03	2.20	0.36
benzene, nitro-	<chem>N(=O)(=O)c(cccc1)c1</chem>	1.85	1.81	-0.04	1.89	0.04
furane, 2-methyl-	<chem>C1=C(C)OC=C1</chem>	1.85	1.91	0.06	1.75	-0.10
benzenamine, 2-nitro-	<chem>N(=O)(=O)c(c(N)ccc1)c1</chem>	1.85	2.02	0.17	1.43	-0.42
ethanol, 2-(hexyloxy)-	<chem>O(CCCCCC)CCO</chem>	1.86	1.55	-0.31	1.82	-0.04
3-pentanone, 2,4-dimethyl-	<chem>O=C(C(C)C)C(C)C</chem>	1.86	1.58	-0.28	1.91	0.05
methane, bromotrifluoro-	<chem>FC(F)(F)Br</chem>	1.86	1.59	-0.27	1.55	-0.31
benzoic acid, 4-amino-, ethyl ester	<chem>O=C(OCC)c(ccc(N)c1)c1</chem>	1.86	1.80	-0.06	2.20	0.34
benzenepropanoic acid, -oxo-, ethyl ester	<chem>O=C(OCC)CC(=O)c(cccc1)c1</chem>	1.87	1.71	-0.16	1.71	-0.16
benzoic acid	<chem>O=C(O)c(cccc1)c1</chem>	1.87	1.87	0.00	1.72	-0.15
2-propenoic acid, 2-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester	<chem>O=C(OCCOCCOCCOC(=O)C(=C)C)C(=C)C</chem>	1.88	1.66	-0.22	1.58	-0.30
2-hexanone, 5-methyl-	<chem>O=C(CCC(C)C)C</chem>	1.88	1.66	-0.22	1.88	0.00
2-propanol, 1-[4-(2-methoxyethyl)phenoxy]-3-[(1-methylethyl)amino]-, 2,3-dihydroxybutanedioate (2:1)	<chem>CC(C)NCC(O)COc1ccc(CCOC)cc1</chem>	1.88	1.69	-0.19	1.80	-0.08
benzenamine, 3-chloro-	<chem>Nc(cccc1Cl)c1</chem>	1.88	1.72	-0.16	1.93	0.05
methanone, phenyl-2-pyridinyl-	<chem>O=C(c(cccc1)c1)c(nc22)c2</chem>	1.88	1.96	0.08	2.13	0.25
benzenepropanol	<chem>OCCcC(cccc1)c1</chem>	1.88	2.06	0.18	2.00	0.12
benzoic acid, 2-amino-, methyl ester	<chem>O=C(OC)c(c(N)ccc1)c1</chem>	1.88	2.26	0.38	1.60	-0.28
pyridine, 2,4,6-trimethyl-	<chem>n(c(cc(c1)C)C)c1C</chem>	1.88	2.45	0.57	2.10	0.22
benzoic acid, 4-nitro-	<chem>O=C(O)c(ccc(N(=O)(=O))c1)c1</chem>	1.89	1.69	-0.20	1.51	-0.38
2,4,6-cycloheptatrien-1-one, 2-hydroxy-4-(1-methylethyl)-	<chem>O=C1C=CC=C(C(C)C)C=C1O</chem>	1.89	1.83	-0.06	1.82	-0.07
ethane, 1,1,2-trichloro-	<chem>ClCC(Cl)Cl</chem>	1.89	2.01	0.12	2.02	0.13
2H-1-benzopyran-2-one, 7-hydroxy-4-methyl-	<chem>c1(O)cc2OC(=O)C=C(C)c2cc1</chem>	1.90	1.58	-0.32	2.19	0.29
benzenamine, 2-chloro-	<chem>Nc(c(ccc1)Cl)c1</chem>	1.90	1.72	-0.18	1.93	0.03
2-propenal, 3-phenyl-	<chem>O=CC=Cc(cccc1)c1</chem>	1.90	1.82	-0.08	2.00	0.10
propane, 2-chloro-	<chem>C(Cl)(C)C</chem>	1.90	2.00	0.10	1.49	-0.41
1,4-naphthalenediol	<chem>Oc(c(c(c(O)c1)ccc2)c2)c1</chem>	1.90	2.21	0.31	1.96	0.06
2,7-naphthalenediol	<chem>Oc(ccc(c1cc(O)c2)c2)c1</chem>	1.90	2.21	0.31	2.03	0.13
benzaldehyde, 2,5-dimethoxy-	<chem>O=Cc(c(OC)ccc1OC)c1</chem>	1.91	1.87	-0.04	1.51	-0.40

phenol, 4-nitro-	N(=O)(=O)c(ccc(O)c1)c1	1.91	1.91	0.00	1.93	0.02
pregna-1,4-diene-3,20-dione, 16,21-bis(acetyloxy)-	O=C1C=C2CCC3C4CC(OC(=O)C)C(C	1.92	1.51	-0.41	2.05	0.13
9-fluoro-11,17-dihydroxy-, (11-beta,16-alpha)-	O) (C(=O)COC(=O)C)C4(C)CC(O)C3(F) C2(C)C=C1					
benzene, (methoxymethyl)-	O(Cc(cccc1)c1)C	1.92	1.77	-0.15	1.69	-0.23
1,4-naphthalenedione, 5-hydroxy-	Oc1cccc2C(=O)C=CC(=O)c12	1.92	1.96	0.04	1.93	0.01
ethanone, 1-(2-hydroxyphenyl)-	O=C(c(c(O)ccc1)c1)C	1.92	1.97	0.05	1.57	-0.35
hexanoic acid	O=C(O)CCCCC	1.92	2.05	0.13	1.88	-0.04
butane, 1,1-[oxybis(2,1-ethanedioxy)]bis-	O(CCOCCOCCOCC)CCCC	1.92	2.46	0.54	2.48	0.56
strychnidin-10-one	O=C(N(c(c(C1(C(N(C2)CC(C3C4C5	1.93	1.85	-0.08	1.68	-0.25
	OC6)=C6)C3)C2)ccc7)c7)C14)C5					
acetic acid, 2-methylphenyl ester	O=C(OC(c(ccc1)C)c1)C	1.93	2.14	0.21	1.96	0.03
pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-	C1=CC(=O)C=C2CCC3C4CC(C)C(O	1.94	1.72	-0.22	1.93	-0.01
trihydroxy-16-methyl-, (11-beta,16-beta)-	)C(=O)CO)C4(C)CC(O)C3(F)C12C					
2-propenoic acid, 2-methyl-, ethyl ester	O=C(OCC)C(=C)C	1.94	1.77	-0.17	1.69	-0.25
phenol, 4-methyl-	Oc(ccc(c1)C)c1	1.94	2.06	0.12	1.95	0.01
benzenamine, 4-methoxy-2-nitro-	N(=O)(=O)c(c(N)ccc1OC)c1	1.94	2.10	0.16	1.61	-0.33
1,5-naphthalenediol	Oc(c(c(c(O)cc1)cc2)c1)c2	1.94	2.21	0.27	1.96	0.02
1,7-naphthalenediol	Oc1ccc2cccc(O)c2c1	1.94	2.21	0.27	2.00	0.06
2-propen-1-ol, 3-phenyl-	OCC=Cc(ccccc1)c1	1.95	1.84	-0.11	1.93	-0.02
ethane, 1,1-thiobis-	S(CC)CC	1.95	1.90	-0.05	2.46	0.51
phenol, 2-methyl-	Oc(c(ccc1)C)c1	1.95	2.06	0.11	1.89	-0.06
2-propenenitrile, 3-phenyl-	C(#N)C=C(c(cccc1)c1	1.96	1.84	-0.12	2.01	0.05
benzoic acid, 4-methoxy-	O=C(O)c(ccc(OC)c1)c1	1.96	1.96	0.00	1.63	-0.33
2,2':6',2'-terpyridine	n(c(ccc1)c(nc(c(ncccc2)c2)cc3)c3)c1	1.96	1.96	0.00	2.78	0.82
benzoic acid, 4-hydroxy-, methyl ester	O=C(OC)c(ccc(O)c1)c1	1.96	2.00	0.04	2.17	0.21
ethane, 1,2-dibromo-	BrCCBr	1.96	2.01	0.05	2.08	0.12
phenol, 3-methyl-	Oc(cccc1C)c1	1.96	2.06	0.10	1.93	-0.03
acetic acid, phenylmethyl ester	O=C(OCc(ccccc1)c1)C	1.96	2.08	0.12	2.07	0.11
benzenamine, 4-ethyl-	Nc(ccc(c1)CC)c1	1.96	2.11	0.15	1.91	-0.05
cyclohexanecarboxylic acid	O=C(O)C(CCCC1)C1	1.96	2.36	0.40	1.88	-0.08
pyrazine, 2-methyl-3-(2-methylpropyl)-	n(c(c(nc1)CC(C)C)C)c1	1.96	2.43	0.47	2.04	0.08
methane, trichloro-	C(Cl)(Cl)Cl	1.97	1.52	-0.45	1.67	-0.30
benzeneethanol, alpha-methyl-	OC(C)Cc(cccc1)c1	1.97	1.98	0.01	1.95	-0.02
1,3-naphthalenediol	Oc(c(c(ccc1)cc2O)c1)c2	1.97	2.21	0.24	2.02	0.05
2(1H)-naphthalenone, octahydro-	O=C(CCC(C1CCC2)C2)C1	1.97	2.49	0.52	2.85	0.88
propane, 1,1,1-triethoxy-	O(C(OC)(OC)CC)CC	1.97	3.10	1.13	1.89	-0.08
7-quinolinol	n(c(c(ccc1O)cc2)c1)c2	1.98	1.66	-0.32	1.93	-0.05
2-heptanone	O=C(CCCCC)C	1.98	1.73	-0.25	1.92	-0.06
benzenemethanamine, N,N-dimethyl-	N(Cc(cccc1)c1)(C)C	1.98	1.75	-0.23	1.84	-0.14
2H-1-benzopyran-2-one, 4-hydroxy-3-[1-(4-	O=C1Oc2cccc2C(O)=C1C(CC(=O)	1.98	2.05	0.07	2.53	0.55
nitrophenyl)-3-oxobutyl]-	C)c3ccc(N(=O)=O)cc3					
phenol, 3-ethoxy-	O(c(cccc1O)c1)CC	1.98	2.08	0.10	1.88	-0.10
benzene, 1-methyl-2,4-dinitro-	N(=O)(=O)c(ccc(c1N(=O)(=O))C)c1	1.98	2.18	0.20	1.90	-0.08
propane, 1,2-dichloro-	ClCC(Cl)C	1.98	2.25	0.27	2.13	0.15
ethanol, 2-(4-chlorophenoxy)-	O(c(ccc(c1)Cl)c1)CCO	1.99	1.74	-0.25	1.91	-0.08
1,3-butadiene	C(C=C)=C	1.99	2.03	0.04	1.94	-0.05
benzene, 1,1-[sulfinylbis(methylene)]bis-	O=S(Cc(cccc1)c1)Cc(cccc2)c2	1.99	2.19	0.20	2.28	0.29
1,4-benzenedicarboxylic acid	O=C(O)c(ccc(c1)C(=O)O)c1	2.00	1.76	-0.24	1.01	-0.99
phenol, 3-nitro-	N(=O)(=O)c(cccc1O)c1	2.00	1.91	-0.09	1.92	-0.08
pregna-1,4-diene-3,20-dione, 9-fluoro-11,17-	CC1CC2C3CCC(O)	2.00	2.06	0.06	2.34	0.34
dihydroxy-6-methyl-, (6-alpha,11)-	(C(=O)C)C3(C)CC(O)C2(F)C4(C)C=					
	CC(=O)C=C14					
ethane, iodo-	C(I)I	2.00	2.08	0.08	2.29	0.29
ethane, hexafluoro-	FC(F)(F)C(F)(F)F	2.00	2.15	0.15	2.46	0.46
benzene, nitroso-	O=Nc(cccc1)c1	2.01	1.86	-0.15	1.41	-0.60
benzothiazole	c1ccc2ncsc2c1	2.01	2.17	0.16	2.13	0.12
8-quinolinol	n(c(c(ccc1)cc2)c1O)c2	2.02	1.66	-0.36	1.91	-0.11
benzoic acid, 3-methoxy-	O=C(O)c(cccc1OC)c1	2.02	1.96	-0.06	1.61	-0.41
cholan-24-oic acid, 3,7,12-trihydroxy-, (3-alpha,5 ,	O=C(O)CCCC(C(C(C(C(C(C(C1)CC	2.02	3.52	1.50	2.26	0.24
7-alpha,12-alpha)-	(O)C2)(C2)C3)C1O)C4) (C3O)C)C4)C					
1H-indazole, 5-nitro-	O=N(=O)c(ccc(NN=C1)c12)c2	2.03	1.05	-0.98	1.54	-0.49
1-hexanol	CCCCCC	2.03	1.82	-0.21	2.03	0.00
2-propanol, 1,1,1-trichloro-2-methyl-	OC(C(Cl)(Cl)Cl)(C)C	2.03	2.09	0.06	2.31	0.28
quinoline	n(c(c(ccc1)cc2)c1)c2	2.03	2.14	0.11	2.19	0.16

benzoic acid, 5-(aminosulfonyl)-4-chloro-2-[(2-furanylmethyl)amino]-	NS(=O)(=O)c2cc(C(=O)(O)c(NC1CCCC1)CC2Cl	2.03	2.32	0.29	2.71	0.68
quinoxaline, 5-methyl-	n(c(c(nc1ccc2)c2C)c1	2.04	1.66	-0.38	1.54	-0.50
benzoic acid, 2-methoxy-, methyl ester	O=C(OC)c(c(OC)ccc1)c1	2.04	1.91	-0.13	2.06	0.02
propane, 1-chloro-	CICCCC	2.04	2.07	0.03	2.09	0.05
benzene, 1,4-dimethoxy-	O(c(cc(OC)c1)c1)C	2.04	2.15	0.11	2.05	0.01
2H-1,4-benzodiazepin-2-one, 7-bromo-1,3-dihydro-	c1c(Br)cc2C(c3ncccc3)=NCC(=O)Nc	2.05	1.93	-0.12	2.09	0.04
5-(2-pyridinyl)-	2c1					
benzoic acid, 2-chloro-	O=C(O)c(c(ccc1)Cl)c1	2.05	2.18	0.13	2.39	0.34
1-hexanamine	NCCCCC	2.06	1.82	-0.24	1.98	-0.08
benzeneethanamine, N-alpha-dimethyl-	CNC(C)Cc1cccc1	2.07	2.22	0.15	2.23	0.16
isoquinoline	n(ccc(c1ccc2)c2)c1	2.08	2.14	0.06	2.14	0.06
7-oxabicyclo[4.1.0]heptane, 3-ethenyl-	O(C1CC(C=C)CC2)C12	2.08	2.43	0.35	1.65	-0.43
acetonitrile, trichloro-	C(#N)C(Cl)(Cl)Cl	2.09	1.21	-0.88	1.80	-0.29
methane, trichloronitro-	N(=O)(=O)C(Cl)(Cl)Cl	2.09	1.32	-0.77	2.10	0.01
acetamide, N-(4-chlorophenyl)-	O=C(Nc(ccc(c1)Cl)c1)C	2.09	1.74	-0.35	1.72	-0.37
ethene, 1,2-dichloro-, (E)-	C(=CCl)Cl	2.09	1.98	-0.11	1.85	-0.24
acetic acid, 3-methylphenyl ester	O=C(OC(cccc1C)c1)C	2.09	2.14	0.05	1.95	-0.14
phenol, 2-(1-methylethoxy)-	O(c(c(O)ccc1)c1)C(C)C	2.09	2.25	0.16	2.27	0.18
ethanol, 2-(ethylphenylamino)-	OCCN(c(cccc1)c1)CC	2.10	1.69	-0.41	1.72	-0.38
2-propanol, 1-[(1-methylethyl)amino]-3-[2-(2-propenyloxy)phenoxy]-	CC(C)NCC(O)COc1c(OCC=C)cccc1	2.10	1.83	-0.27	2.44	0.34
2,4,6(1H,3H,5H)-pyrimidinetrione, 5-ethyl-5-(1-methylbutyl)-	CCCC(C)C1(CC(C(=O)NC(=O)NC1=O	2.10	2.00	-0.10	2.16	0.06
pregn-4-ene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-	CC(=O)OCC(=O)C3(O)CCC4C2CCC1=CC(=O)CCC1(C)C2C(=O)CC34C	2.10	2.14	0.04	2.35	0.25
propane, 1-bromo-	BrCCC	2.10	2.16	0.06	2.18	0.08
benzene, 2-methyl-1,3-dinitro-	N(=O)(=O)c(c(c(N(=O)=O)cc1)C)c1	2.10	2.18	0.08	1.81	-0.29
ethanone, 1-(4-methylphenyl)-	O=C(c(ccc(c1)C)c1)C	2.10	2.22	0.12	2.11	0.01
2,4(1H,3H)-pyrimidinedione, 5-bromo-6-methyl-3-(1-methylpropyl)-	N1C(=O)N(C(C)CC)C(=O)C(Br)=C1C	2.11	1.68	-0.43	1.20	-0.91
benzene, (2-nitroethenyl)-	N(=O)(=O)C=Cc(cccc1)c1	2.11	1.95	-0.16	2.17	0.06
benzene, methoxy-	O(c(cccc1)c1)C	2.11	2.07	-0.04	2.10	-0.01
acetic acid, 4-methylphenyl ester	O=C(OC(ccc(c1)C)c1)C	2.11	2.14	0.03	1.96	-0.15
benzoic acid, methyl ester	O=C(OC)c(cccc1)c1	2.12	1.83	-0.29	1.98	-0.14
phenol, 2-methyl-4,6-dinitro-	N(=O)(=O)c(cc(N(=O)=O)c(O)c1C)c1	2.12	2.27	0.15	2.09	-0.03
4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-1-methyl-6-phenyl-	c1cc2n3c(C)nnc3CN=C(c4cccc4)c2cc1Cl	2.12	3.87	1.75	2.23	0.11
ethanone, 2-hydroxy-1,2-diphenyl-	O=C(c(cccc1)c1)C(O)c(cccc2)c2	2.13	1.84	-0.29	2.64	0.51
benzene	c(cccc1)c1	2.13	1.99	-0.14	2.03	-0.10
2-propenoic acid, 3-phenyl-	O=C(O)C=Cc(cccc1)c1	2.13	2.07	-0.06	2.38	0.25
ethene, 1,1-dichloro-	C=C)(Cl)Cl	2.13	2.12	-0.01	1.97	-0.16
1H-indole	c1ccc2ccnc2c1	2.14	2.05	-0.09	2.29	0.15
propane, 2-bromo-	BrC(C)C	2.14	2.08	-0.06	1.83	-0.31
phenol, 2-chloro-	Oc(c(ccc1)Cl)c1	2.15	2.16	0.01	2.40	0.25
benzenamine, N,4-dimethyl-	N(c(ccc(c1)C)c1)C	2.15	2.17	0.02	2.10	-0.05
methane, dichlorodifluoro-	FC(F)(Cl)Cl	2.16	1.82	-0.34	2.06	-0.10
threo-alpha-galacto-octopyranoside, methyl 7-chloro-6,7,8-trideoxy-6-[[[1-methyl-4-propyl-2-pyrrolidinyl]carbonyl]amino]-1-thio-	CCCC1CC(N(C)C1)C(=O)NC(C(C)Cl)C2OC(SC)C(O)C(O)C2O	2.16	2.01	-0.15	1.76	-0.40
benzene, (ethoxymethyl)-	O(Cc(cccc1)c1)CC	2.16	2.27	0.11	2.38	0.22
benzene, 1-chloro-2,4-dinitro-	N(=O)(=O)c(ccc(c1N(=O)=O)Cl)c1	2.17	2.27	0.10	2.29	0.12
spiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione, 7-chloro-2',4,6-trimethoxy-6'-beta-methyl-	COc1c(Cl)c2OC(C(OC)=C3)(C(C)CC3=O)C(=O)c2c(OC)c1	2.18	1.92	-0.26	2.71	0.53
3-buten-2-one, 4-phenyl-	O=C(C=Cc(cccc1)c1)C	2.18	2.04	-0.14	2.23	0.05
benzamide, N,N-diethyl-3-methyl-	O=C(N(CC)CC)c(cccc1C)c1	2.18	2.26	0.08	2.10	-0.08
propane, 1-bromo-3-chloro-	BrCCCCl	2.18	2.41	0.23	2.12	-0.06
cyclohexanone, 2-(2-chlorophenyl)-2-(methylamino)-	C1(=O)C(NC)(c2c(Cl)cccc2)CCCC1	2.18	3.12	0.94	2.69	0.51
2H-1,4-benzodiazepin-2-one, 7-chloro-1,3-dihydro-	CN2C(=O)C(O)N=C(c1cccc1)c3cc(Cl)ccc23	2.19	2.15	-0.04	2.16	-0.03
3-hydroxy-1-methyl-5-phenyl-	O=C(c(cccc1)c1)CC	2.19	2.16	-0.03	2.15	-0.04
1-propanone, 1-phenyl-	C1C(=O)C=C2CCC3C4CCC(O)(C(=O)COC(=O)C)C4(C)CC(O)C3C2(C)C1	2.19	2.36	0.17	2.31	0.12
pregn-4-ene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11)-						
1,4-naphthalenedione, 2-methyl-	c1cc2C(=O)C=C(C)C(=O)c2cc1	2.20	2.21	0.01	1.91	-0.29

3,5-pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-, dimethyl ester	<chem>COC(=O)C1=C(C)NC(=C(C1c2ccccc2N(=O)C(=O)C(=O)OC)C</chem>	2.20	2.50	0.30	2.49	0.29
benzene, 1,3-dimethoxy-4-heptanol	<chem>O(c(cccc1OC)c1)C</chem>	2.21	2.15	-0.06	2.00	-0.21
propanenitrile, 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methyl-bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-2,3-naphthalenediol	<chem>OC(CCC)CCC</chem>	2.22	2.24	0.02	2.26	0.04
3-heptanol	<chem>CCNc1nc(Cl)nc(NC(C)(C)C(#N))n1</chem>	2.22	2.51	0.29	2.05	-0.17
2H-1,4-benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-5-phenyl-1-naphthaleneacetic acid	<chem>O=C(C=C(C)C12)C(C2)C1(C)C</chem>	2.23	3.21	0.98	2.30	0.07
1,4-benzenedicarboxylic acid, dimethyl ester	<chem>Oc(c(O)cc(c1ccc2)c2)c1</chem>	2.24	2.21	-0.03	2.08	-0.16
1-naphthalenamine	<chem>OC(CCCC)CC</chem>	2.24	2.24	0.00	2.29	0.05
2H-1,4-benzodiazepin-2-one, 1,3-dihydro-7-nitro-5-phenyl-benzenamine, 4-bromo-benzoic acid, 2-hydroxy-benzoic acid, anhydride	<chem>OC3N=C(c1ccccc1)c2cc(Cl)ccc2NC3(=O)</chem>	2.24	2.32	0.08	2.01	-0.23
benzoic acid, 4-methoxy-, methyl ester	<chem>O=C(O)Cc(c(c(ccc1)cc2)c1)c2</chem>	2.24	2.60	0.36	2.97	0.73
2-propenoic acid, 2-methyl-, 2-hydroxy-3-phenoxypropyl ester	<chem>O=C(OC)c(ccc(c1)C(=O)OC)c1</chem>	2.25	1.66	-0.59	1.83	-0.42
benzenesulfonamide, 4-chloro-N-[(propylamino)carbonyl]-3-pyridinecarboxylic acid, butyl ester	<chem>c(c(c(N)cc1)ccc2)(c2)c1</chem>	2.25	2.25	0.00	2.27	0.02
benzene, fluoro-benzoic acid, 4-methyl-propane, 1,2,3-trichloro-phenol, 2-methoxy-4-(2-propenyl)-2-naphthalenamine	<chem>O=C3CN=C(c1ccccc1)c2cc(ccc2N3)N(=O)=O</chem>	2.25	2.45	0.20	1.95	-0.30
1-butanethiol	<chem>Nc(ccc(c1)Br)c1</chem>	2.26	1.97	-0.29	2.10	-0.16
2-naphthalenol, 1-nitroso-benzeneacetic acid, ethyl ester	<chem>O=C(O)c(c(O)ccc1)c1</chem>	2.26	2.24	-0.02	1.96	-0.30
acetamide, N-(4-bromophenyl)-pyrazine, 2-methyl-6-propoxy-3,5-pyrazolidinedione, 1,2-diphenyl-4-[2-(phenylsulfinyl)ethyl]-benzeneacetic acid, alpha-hydroxy-alpha-phenyl-ethane, 2-bromo-2-chloro-1,1,1-trifluoro-acetic acid, pentyl ester	<chem>O=C(OC(=O)c(ccc1)c1)c(cccc2)c2</chem>	2.26	2.33	0.07	3.22	0.96
methane, diiodo-benzene, 1-methyl-2-nitro-acetic acid, 2-phenylethyl ester	<chem>O=C(OC)c(ccc(OC)c1)c1</chem>	2.27	1.91	-0.36	2.05	-0.22
phenol, 2,4-dimethyl-benzene, chloromethyl-1H-indole-3-butanoic acid	<chem>C=C(C)C(=O)OCC(O)COc1ccccc1</chem>	2.27	1.96	-0.31	1.83	-0.44
1H-indole-2-carboxylic acid	<chem>c1cc(Cl)ccc1S(=O)(=O)NC(=O)NCCC</chem>	2.27	2.01	-0.26	2.15	-0.12
benzenamine, N,N-dimethyl-2-heptanol	<chem>O=C(OCCC)c(cccn1)c1</chem>	2.27	2.11	-0.16	2.23	-0.04
ethanone, 1-(4-chlorophenyl)-benzenepropanoic acid, methyl ester	<chem>Fc(cccc1)c1</chem>	2.27	2.19	-0.08	2.18	-0.09
2-butene	<chem>O=C(O)c(ccc(c1)C)c1</chem>	2.27	2.42	0.15	2.12	-0.15
8-quinolinol, 2-methyl-benzaldehyde, 2-chloro-thiophene, 2-methyl-butane, 2-chloro-phenol, 2,5-dimethyl-1H-2,1,3-benzothiadiazin-4(3H)-one, 3-(1-methylethyl)-, 2,2-dioxide	<chem>C1CC(Cl)CCl</chem>	2.27	2.50	0.23	2.29	0.02
1-propene, 2-methyl-benzenamine, 4-iodo-thiophene, 3-methyl-benzenesulfonamide, N-[(butylamino)carbonyl]-4-methyl-[1,1-biphenyl]-4,4-diamine, 3,3-dimethyl-benzenebutanol	<chem>O(c(c(O)ccc1CC=C)c1)C</chem>	2.27	2.73	0.46	2.66	0.39
phenol, 3,5-dimethyl-	<chem>c(c(ccc1N)ccc2)(c2)c1</chem>	2.28	2.25	-0.03	2.30	0.02
	<chem>SCCCC</chem>	2.28	2.25	-0.03	2.51	0.23
	<chem>O=Nc(c(c(ccc1)cc2)c1)c2O</chem>	2.28	2.56	0.28	2.50	0.22
	<chem>O=C(OCC)Cc(cccc1)c1</chem>	2.28	2.57	0.29	2.48	0.20
	<chem>O=C(Nc(ccc(c1)Br)c1)C</chem>	2.29	1.99	-0.30	1.88	-0.41
	<chem>n1c(C)cncc1OCCC</chem>	2.29	2.45	0.16	2.08	-0.21
	<chem>O=C2C(CCS(=O)c1ccccc1)C(=O)N(N2c3ccccc3)c4ccccc4</chem>	2.30	2.14	-0.16	2.92	0.62
	<chem>O=C(O)C(O)(c(cccc1)c1)c(cccc2)c2</chem>	2.30	2.24	-0.06	2.12	-0.18
	<chem>FC(F)(F)C(Cl)Br</chem>	2.30	2.26	-0.04	2.50	0.20
	<chem>O=C(OCCCC)C</chem>	2.30	2.34	0.04	2.46	0.16
	<chem>C(I)I</chem>	2.30	2.35	0.05	2.25	-0.05
	<chem>N(=O)(=O)c(c(ccc1)C)c1</chem>	2.30	2.36	0.06	2.32	0.02
	<chem>O=C(OCCc(cccc1)c1)C</chem>	2.30	2.57	0.27	2.38	0.08
	<chem>Oc(c(cc(c1)C)C)c1</chem>	2.30	2.61	0.31	2.37	0.07
	<chem>ClCc1ccccc1</chem>	2.30	2.79	0.49	2.51	0.21
	<chem>O=C(O)CCCC(c(c(N1)ccc2)c2)=C1</chem>	2.30	2.84	0.54	2.38	0.08
	<chem>c1ccc2cc(C(=O)O)nc2c1</chem>	2.31	1.94	-0.37	1.79	-0.52
	<chem>N(c(cccc1)c1)(C)C</chem>	2.31	2.17	-0.14	2.05	-0.26
	<chem>OC(CCCCC)C</chem>	2.31	2.24	-0.07	2.34	0.03
	<chem>O=C(c(ccc(c1)Cl)c1)C</chem>	2.32	2.32	0.00	2.41	0.09
	<chem>O=C(OC)CCc(cccc1)c1</chem>	2.32	2.57	0.25	2.35	0.03
	<chem>C(=CC)C</chem>	2.33	2.09	-0.24	2.32	-0.01
	<chem>n(c(c(ccc1)cc2)c1O)c2C</chem>	2.33	2.21	-0.12	2.52	0.19
	<chem>O=Cc(c(ccc1)Cl)c1</chem>	2.33	2.35	0.02	2.23	-0.10
	<chem>C1=C(C)SC=C1</chem>	2.33	2.36	0.03	2.30	-0.03
	<chem>C(Cl)(CC)C</chem>	2.33	2.49	0.16	2.34	0.01
	<chem>Oc(c(ccc1)C)c1</chem>	2.33	2.61	0.28	2.35	0.02
	<chem>O=C(N(S(=O)(=O)Nc1cccc2)C(C)C)c12</chem>	2.34	1.67	-0.67	1.86	-0.48
	<chem>C(=C)(C)C</chem>	2.34	2.23	-0.11	1.87	-0.47
	<chem>Nc(ccc(c1)I)c1</chem>	2.34	2.24	-0.10	2.58	0.24
	<chem>C1(C)=CSC=C1</chem>	2.34	2.36	0.02	2.28	-0.06
	<chem>O=C(NCCCC)NS(=O)(=O)c(c(ccc1)C)c1</chem>	2.34	2.41	0.07	2.04	-0.30
	<chem>Nc1c(C)cc(c2cc(C)C(N)cc2)cc1</chem>	2.34	3.02	0.68	2.44	0.10
	<chem>OCCCCc(cccc1)c1</chem>	2.35	2.55	0.20	2.45	0.10
	<chem>Oc(cc(cc1)C)C1</chem>	2.35	2.61	0.26	2.38	0.03

propane	C(C)C	2.36	1.81	-0.55	2.19	-0.17
2-propenoic acid, butyl ester	O=C(OCCCC)C=C	2.36	2.20	-0.16	2.20	-0.16
butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethylester	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC	2.36	2.29	-0.07	2.67	0.31
phenol, 2,6-dimethyl-	Oc(c(ccc1)C)c1C	2.36	2.61	0.25	2.32	-0.04
2-octanone	O=C(CCCCCC)C	2.37	2.22	-0.15	2.54	0.17
benzene, 1-methyl-4-nitro-	N(=O)(=O)c(ccc(c1)C)c1	2.37	2.36	-0.01	2.34	-0.03
benzoic acid, 3-methyl-	O=C(O)c(cccc1C)c1	2.37	2.42	0.05	2.08	-0.29
propane, 1,3-dibromo-	BrCCBr	2.37	2.50	0.13	2.55	0.18
androst-4-en-3-one, 9-fluoro-11,17-dihydroxy-17-methyl-, (11-beta,17-beta)-	CC1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3(F)C(O)CC21C	2.38	2.49	0.11	2.50	0.12
bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-	O=C(C(C(C1C2)(C)C)(C2)C)C1	2.38	3.04	0.66	2.85	0.47
phenol, 4-chloro-	Oc(ccc(c1)Cl)c1	2.39	2.16	-0.23	2.37	-0.02
ethane, 1,1,2,2-tetrachloro-	C(C(Cl)Cl)(Cl)Cl	2.39	2.19	-0.20	2.57	0.18
benzoic acid, 2-mercapto-	O=C(O)c(c(S)ccc1)c1	2.39	2.22	-0.17	1.65	-0.74
2H-1,4-benzodiazepin-2-one, 7-chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-	OC3N=C(c1ccccc1Cl)c2cc(Cl)ccc2N3=O	2.39	2.41	0.02	2.98	0.59
benzene, 1-chloro-4-nitro-	N(=O)(=O)c(ccc(c1)Cl)c1	2.39	2.46	0.07	2.56	0.17
methane, tribromo-	BrC(Br)Br	2.40	1.79	-0.61	2.50	0.10
pregna-1,4-diene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11 -)	O=C1C=C2CCC3C4CCC(O)(C(=O)COC(=O)C)C4(C)CC(O)C3C2(C)C=C1	2.40	2.14	-0.26	2.17	-0.23
butene	C=CCC	2.40	2.17	-0.23	2.21	-0.19
furan, 2-ethyl-	C1=COC(CC)=C1	2.40	2.40	0.00	2.50	0.10
phenol, 3-ethyl-	Oc1cc(CC)ccc1	2.40	2.55	0.15	2.53	0.13
benzoic acid, 2-iodo-	O=C(O)c(c(ccc1)I)c1	2.40	2.70	0.30	2.51	0.11
2H-1,4-benzodiazepin-2-one, 5-(2-chlorophenyl)-1,3-dihydro-7-nitro-	Clc1ccccc1C2=NCC(=O)Nc3ccc(cc23)N(=O)=O	2.41	2.53	0.12	2.76	0.35
urea, N'-(3-chloro-4-methylphenyl)-N,N-dimethyl-	CN(C)C(=O)Nc1ccc(C)c(Cl)c1	2.41	2.58	0.17	2.25	-0.16
ethene, trichloro-	C=CCl(Cl)Cl	2.42	2.47	0.05	2.45	0.03
heptanoic acid	O=C(O)CCCCC	2.42	2.54	0.12	2.41	-0.01
1,3-butadiene, 2-methyl-	C(C=C)=C(C)C	2.42	2.58	0.16	2.22	-0.20
1,2-benzenedicarboxylic acid, diethyl ester	O=C(OCC)c(c(ccc1)C(=O)OCC)c1	2.42	2.65	0.23	2.60	0.18
benzenebutanoic acid	O=C(O)CCCCc(cccc1)c1	2.42	2.78	0.36	2.29	-0.13
2(3H)-benzothiazolethione	N(c(c(S1)ccc2)c2)=C1S	2.42	2.86	0.44	2.37	-0.05
4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-	c1cc2n3c(C)nnc3CN=C(c4c(Cl)cccc4)c2cc1Cl	2.42	3.96	1.54	2.94	0.52
2-furanmethanol, 5-ethenyltetrahydro-alpha,alpha-5-trimethyl-	O(C(C=C)(CC1)C)C1C(O)(C)C	2.43	1.99	-0.44	1.51	-0.92
acetamide, 2-(diethylamino)-N-(2,6-dimethylphenyl)-	O=C(Nc(c(ccc1)C)c1C)CN(CC)CC	2.44	1.66	-0.78	1.81	-0.63
3H-1,4-benzodiazepin-2-amine, 7-chloro-N-methyl-5-phenyl-, 4-oxide	CNC2=Nc1ccc(Cl)cc1C(=N(=O)C2)c3ccccc3	2.44	2.42	-0.02	2.01	-0.43
1,3-pentadiene	C(=CC=C)C	2.44	2.45	0.01	2.65	0.21
benzenemethanol, 4-methyl-, acetate	O=C(OCCc(ccc(c1)C)c1)C	2.44	2.63	0.19	2.71	0.27
5H-dibenz[b,f]azepine-5-carboxamide	NC(=O)N2c1ccccc1C=Cc3ccccc23	2.45	2.25	-0.20	2.10	-0.35
benzene, 1-methyl-3-nitro-	N(=O)(=O)c(ccc1C)c1	2.45	2.36	-0.09	2.32	-0.13
3(2H)-isothiazolone, 2-octyl-	O=C1C=CSN1CCCCCCCC	2.45	2.61	0.16	3.77	1.32
estra-1,3,5(10)-triene-3,16,17-triol, (16-alpha,17 -)	CC34CCC1C(CCc2cc(O)ccc12)C3C(C(O)C4O	2.45	2.81	0.36	2.54	0.09
benzoic acid, 2-methyl-	O=C(O)c(c(ccc1)C)c1	2.46	2.08	-0.38	2.03	-0.43
phenol, 4-chloro-2-nitro-	N(=O)(=O)c(c(O)ccc1Cl)c1	2.46	2.55	0.09	2.56	0.10
2,4-imidazolidinedione, 5,5-diphenyl-	O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3	2.47	2.16	-0.31	2.26	-0.21
benzoic acid, 4-hydroxy-, ethyl ester	O=C(OCC)c(ccc(O)c1)c1	2.47	2.49	0.02	2.76	0.29
phenol, 2-ethyl-	Oc(c(ccc1)CC)c1	2.47	2.55	0.08	2.45	-0.02
1,4-pentadiene	C(=C)CC=C	2.48	2.52	0.04	2.39	-0.09
pregna-1,4-diene-3,20-dione, 6,9-difluoro-11,21-dihydroxy-16,17-[(1-methylethylidene)bis(oxy)]-, (6-alpha,1-beta,1-alpha)-	C1(=O)C=C2C(F)CC3C4CC5C(C(=O)CO)(OC(C)(C)O5)C4(C)CC(O)C3(F)C2(C)C=C1	2.48	2.56	0.08	2.47	-0.01
phenol, 2,3-dimethyl-	Oc(c(c(cc1)C)C)c1	2.48	2.61	0.13	2.34	-0.14
4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3-(2-chlorophenyl)-5-methyl-4-isoxazolyl]carbonyl]amino]-3,3-dimethyl-7-oxo-	N12C(=O)C(NC(=O)C4=C(C)ON=C4c3c(Cl)cccc3)C1SC(C)(C)C2C(=O)O	2.48	3.22	0.74	2.61	0.13
ethane, 1,1,1-trichloro-	C(Cl)(Cl)(Cl)C	2.49	2.68	0.19	2.45	-0.04
phenol, 3-chloro-	Oc(cccc1Cl)c1	2.50	2.16	-0.34	2.35	-0.15
benzenepropanoic acid, alpha-acetyl-, ethyl ester	CCOC(=O)C(Cc1ccccc1)C(=O)C	2.52	1.92	-0.60	2.15	-0.37

benzenethiol	Sc(ccccc1)c1	2.52	2.69	0.17	2.26	-0.26
butane, 2-chloro-2-methyl-	C(CC)(Cl)(C)C	2.52	2.94	0.42	2.95	0.43
methane, trichlorofluoro-	FC(Cl)(Cl)Cl	2.53	2.13	-0.40	2.25	-0.28
1-butene, 4-bromo-	BrCCC=C	2.53	2.51	-0.02	2.24	-0.29
2-propenoic acid, 2-methyl-, phenylmethyl ester	O=C(OCc(cccc1)c1)C(=C)C	2.53	2.98	0.45	2.86	0.33
thiophene, 2-chloro-	C1=CC=C(Cl)S1	2.54	2.46	-0.08	2.50	-0.04
benzoic acid, 2-hydroxy-, methyl ester	O=C(OC)c(c(O)ccc1)c1	2.55	2.60	0.05	2.07	-0.48
phenol, 4-ethyl-, acetate	CC(=O)Oc1ccc(CC)cc1	2.56	2.63	0.07	2.62	0.06
1-heptanamine	NCCCCCCC	2.57	2.31	-0.26	2.57	0.00
quinoline, 6-methyl-	n(c(c(cc1)C)cc2)c1c2	2.57	2.69	0.12	2.57	0.00
benzoic acid, 2-amino-, ethyl ester	O=C(OC)c(c(N)ccc1)c1	2.57	2.76	0.19	1.95	-0.62
phenol, 4-ethyl-	OC(ccc1)CCc1	2.58	2.55	-0.03	2.54	-0.04
quinoline, 2-methyl-	n(c(c(ccc1)cc2)c1)c2C	2.59	2.69	0.10	2.66	0.07
2-propanol, 1-chloro-, phosphate (3:1)	O=P(OC(CCl)C)(OC(CCl)C)OC(CCl)C	2.59	2.89	0.30	2.83	0.24
2H-1-benzopyran-2-one, 4-hydroxy-3-(3-oxo-1-phenylbutyl)-	c1ccc2C(O)=C(C(c3ccccc3)CC(=O)C)C(=O)Oc2c1	2.60	2.23	-0.37	2.41	-0.19
1H-indole, 3-methyl-	c1ccc2c(C)cnc2c1	2.60	2.60	0.00	2.58	-0.02
quinoline, 8-methyl-	n(c(c(ccc1)cc2)c1)C2	2.60	2.69	0.09	2.53	-0.07
quinoline, 4-methyl-	n(c(c(c1)C)ccc2)c2c1	2.61	2.69	0.08	2.56	-0.05
1,3,5-triazine-2,4-diamine, 6-chloro-N-ethyl-N'-(1-methylethyl)-	n(c(nc1)NC(C)C)NCCc1Cl	2.61	2.82	0.21	2.70	0.09
1-heptanol	OCCCCCCC	2.62	2.31	-0.31	2.53	-0.09
2-propenoic acid, 3-phenyl-, methyl ester	O=C(OC)C=Cc(cccc1)c1	2.62	2.36	-0.26	2.58	-0.04
benzamide, N-phenyl-	O=C(Nc(cccc1)c1)c(cccc2)c2	2.62	2.70	0.08	2.43	-0.19
benzoic acid, ethyl ester	O=C(OC)c(cccc1)c1	2.64	2.32	-0.32	2.39	-0.25
butane, 1-chloro-	ClCCCC	2.64	2.56	-0.08	2.37	-0.27
hexanoic acid, 2-ethyl-	O=C(O)C(CCCC)CC	2.64	2.96	0.32	2.61	-0.03
1H-imidazole, 4,5-dihydro-2-(phenylmethyl)-	c1ccccc1CC2=NCCN2	2.65	2.34	-0.31	2.05	-0.60
phenol, 2-iodo-	OC(c(ccc1)I)c1	2.65	2.68	0.03	2.92	0.27
benzene, 1-methoxy-4-methyl-	O(c(ccc1)C)c1C	2.66	2.62	-0.04	2.63	-0.03
2-propenoic acid, 2-methyl-, 2-methylpropyl ester	O=C(OC(C)C)C(=C)C	2.66	2.67	0.01	2.49	-0.17
benzofuran	c1ccc2ccoc2c1	2.67	2.54	-0.13	2.75	0.08
2-butene, 2-methyl-	C(=CC)C	2.67	2.64	-0.03	2.70	0.03
benzenemethanol, alpha-phenyl-	OC(c(cccc1)c1)c(cccc2)c2	2.67	2.71	0.04	2.76	0.09
phenol, 2,3,6-trimethyl-	OC(c(ccc1)C)c1C	2.67	3.15	0.48	2.72	0.05
benzenemethanamine, N-(phenylmethyl)-	N(Cc(cccc1)c1)Cc(cccc2)c2	2.67	3.24	0.57	2.82	0.15
2-propenoic acid, 3-(4-methoxyphenyl)-	O=C(O)C=Cc(ccc(OC)c1)c1	2.68	2.15	-0.53	2.37	-0.31
benzoic acid, 3-chloro-	O=C(O)c(cccc1Cl)c1	2.68	2.52	-0.16	2.24	-0.44
urea, N'-(3,4-dichlorophenyl)-N,N-dimethyl-	O=C(N(C)C)Nc(ccc(c1Cl)Cl)c1	2.68	2.67	-0.01	2.92	0.24
cinchon-9-ol	OC(c(c(c(nc1)ccc2)c2)c1)C(N(CCC3C4C=C)C4)C3	2.68	3.21	0.53	3.20	0.52
benzenamine, 3,4-dichloro-	Nc(ccc(c1Cl)Cl)c1	2.69	2.37	-0.32	2.74	0.05
2,4-pyrimidinediamine, 5-(4-chlorophenyl)-6-ethyl-	CCc1nc(N)nc(N)c1c2ccc(Cl)cc2	2.69	2.41	-0.28	2.62	-0.07
acetamide, N-(4-bromo-3-chloro-2-methylphenyl)-	CC(=O)Nc1c(Cl)c(Cl)c(Br)cc1	2.69	2.62	-0.07	2.88	0.19
bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-	OC(C(C(C1C2)(C)C)(C2)C)C1	2.69	2.85	0.16	2.83	0.14
benzoic acid, 4-methyl-, methyl ester	O=C(OC)c(ccc(c1)C)c1	2.70	2.38	-0.32	2.47	-0.23
2-naphthalenol	OC(ccc(c1ccc2)c2)c1	2.70	2.69	-0.01	2.93	0.23
1,5-benzothiazepin-4(5H)-one, 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-	c1ccc2N(CCN(C)C)C(=O)C(OC(=O)C)C(c3ccc(OC)cc3)Sc2c1	2.70	2.79	0.09	3.09	0.39
2-cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)-	O=C(C(=CCC1C(=C)C)C)C1	2.71	3.07	0.36	2.77	0.06
2(3H)-furanone, 5-hexyldihydro-	O=C(OC(C1)CCCCC)C1	2.72	2.57	-0.15	3.52	0.80
benzenamine, 4-chloro-2-nitro-	N(=O)(=O)c(c(N)ccc1Cl)c1	2.72	2.66	-0.06	2.06	-0.66
4-piperidinecarboxylic acid, 1-methyl-4-phenyl-, ethyl ester	C1CN(C)CCC1(c2ccccc2)C(=O)OCC	2.72	3.03	0.31	2.90	0.18
3,5-pyrazolidinedione, 4-butyl-1-(4-hydroxyphenyl)-2-phenyl-	CCCCC1C(=O)N(N(C1=O)c2ccc(O)c2)c3ccccc3	2.72	3.04	0.32	2.79	0.07
yohimban-16-alpha-carboxylic acid, 17-alpha-hydroxy-, methyl ester	COC(=O)C4C(O)CCC5CN3CCc1c(nc2ccccc12)C3CC45	2.73	2.11	-0.62	2.36	-0.37
benzene, methyl-	c(cccc1)(c1)C	2.73	2.54	-0.19	2.56	-0.17
benzenepropanoic acid, ethyl ester	O=C(OC)CCc(cccc1)c1	2.73	3.06	0.33	2.79	0.06
phenol, 2,4,6-trimethyl-	OC(c(cc1)C)C)c1C	2.73	3.15	0.42	2.72	-0.01
benzene, 1-methoxy-2-methyl-	O(c(c(ccc1)C)c1)C	2.74	2.62	-0.12	2.60	-0.14
2-oxabicyclo[2.2.2]octane, 1,3,3-trimethyl-	O(C(CCC1C2)(C2)C)C1(C)C	2.74	3.13	0.39	3.36	0.62
thiourea, N,N-dibutyl-	N(C(=S)NCCCC)CCCC	2.75	2.57	-0.18	2.62	-0.13
butane, 1-bromo-	BrCCCC	2.75	2.65	-0.10	2.73	-0.02

thiophene, 2-bromo-	<chem>C1=CC=C(Br)S1</chem>	2.75	2.70	-0.05	2.60	-0.15
octanenitrile	<chem>C(#N)CCCCCCC</chem>	2.75	2.80	0.05	2.76	0.01
pentanoic acid, 2-propyl-	<chem>CCCC(CCC)C(O)=O</chem>	2.75	2.96	0.21	2.54	-0.21
propane, 2-methyl-	<chem>C(C)(C)C</chem>	2.76	2.23	-0.53	2.16	-0.60
pregna-1,4-diene-3,20-dione, 21-(acetyloxy)-9-fluoro-11,17-dihydroxy-16-methyl-, (11-beta,16-beta)-	<chem>CC4CC3C2CCC1=CC(=O)C=CC1(C)C2(F)C(O)CC3(C)C4(O)C(=O)COC(C)=O</chem>	2.77	2.46	-0.31	2.60	-0.17
1-butanone, 1-phenyl-	<chem>O=C(c(cccc1)c1)CCC</chem>	2.77	2.66	-0.11	2.55	-0.22
benzenebutanoic acid, methyl ester	<chem>COC(=O)CCCc1ccccc1</chem>	2.77	3.06	0.29	2.89	0.12
benzenamine, 2,4-dichloro-	<chem>Nc(c(cc1)Cl)Cl)c1</chem>	2.78	2.37	-0.41	2.73	-0.05
1H-pyrrole-2-acetic acid, 1-methyl-5-(4-methylbenzoyl)-	<chem>Cc1ccc(cc1)C(=O)c2ccc(CC(O)=O)nc2C</chem>	2.79	2.56	-0.23	2.81	0.02
methanone, diphenyl-, hydrazone	<chem>N(N)=C(c(cccc1)c1)c(cccc2)c2</chem>	2.79	3.31	0.52	3.23	0.44
1(3H)-isobenzofuranone, 3-butyl-	<chem>O=C(OC(c1cccc2)CCCC)c12</chem>	2.80	2.61	-0.19	3.00	0.20
1H-isindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-	<chem>O=C(N(SCl)C(Cl)C(=O)C1CC=CC2)C12</chem>	2.80	2.74	-0.06	3.00	0.20
alpha-glucopyranosiduronic acid, (3,20)-20-carboxy-11-oxo-30-norolean-12-en-3-yl 2-o-glucopyranuronosyl-	<chem>O1C(C(=O)O)C(O)C(O)C(O)C1OC2C(O)C(O)C(C(=O)O)OC2OC3C(C)(C)C4CCC5(C)C6(C)CCC7(C)CCC(C)(C(=O)O)CC7C6=CC(=O)C5C4(C)CC3</chem>	2.80	3.19	0.39	2.78	-0.02
cholan-24-oic acid, 3,6,7-trihydroxy-, (3-alpha,5,6-alpha,7-alpha)-	<chem>C1C(O)CC2C(O)C(O)C3C4CCC(C(C)CCC(=O)O)C4(C)CCC3C2(C)C1</chem>	2.80	3.52	0.72	2.16	-0.64
acetic acid, (2,4-dichlorophenoxy)-	<chem>O=C(O)COc(c(cc1)Cl)Cl)c1</chem>	2.81	2.62	-0.19	2.82	0.01
benzenamine, N,N,4-trimethyl-	<chem>N(c(ccc1)C)c1(C)C</chem>	2.81	2.72	-0.09	2.58	-0.23
2H-1,4-benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-	<chem>O=C(N(c(c(cc1)Cl)C(=N2)c(cccc3)c3c1)C)C2</chem>	2.82	2.70	-0.12	2.63	-0.19
1-hexanamine, 2-ethyl-	<chem>NCC(CCCC)CC</chem>	2.82	2.73	-0.09	3.10	0.28
ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-	<chem>FC(F)(C(F)F)Cl)Cl</chem>	2.82	2.78	-0.04	2.57	-0.25
prosta-5,13-dien-1-oic acid, 11,15-dihydroxy-9-oxo-	<chem>CCCCC(O)C=CC1C(O)CC(=O)C1CC=CCCC(=O)O</chem>	2.82	3.52	0.70	3.31	0.49
methane, tetrachloro-	<chem>C(Cl)(Cl)(Cl)Cl</chem>	2.83	2.44	-0.39	2.64	-0.19
carbamic acid, (5-benzoyl-1h-benzimidazol-2-yl)-, methyl ester	<chem>c1c(C(=O)c3ccccc3)cc2nc(NC(=O)OC)n(H)c2c1</chem>	2.83	2.71	-0.12	2.67	-0.16
1-butanamine, N-butyl-	<chem>N(CCCC)CCCC</chem>	2.83	2.77	-0.06	2.71	-0.12
urea, N-(2-chloroethyl)-N'-cyclohexyl-N-nitroso-	<chem>CICCN(N=O)C(=O)NC1CCCCC1</chem>	2.83	2.96	0.13	2.62	-0.21
benzene, chloro-	<chem>c(cccc1)(c1)Cl</chem>	2.84	2.64	-0.20	2.78	-0.06
propane, 2,2-thiobis-	<chem>S(C(C)C)C(C)C</chem>	2.84	2.74	-0.10	3.01	0.17
1-naphthalenol	<chem>Oc(c(c(ccc1)cc2)c1)c2</chem>	2.85	2.69	-0.16	2.79	-0.06
benzenamine, N,N,2-trimethyl-	<chem>N(c(c(ccc1)C)c1)(C)C</chem>	2.85	2.72	-0.13	2.56	-0.29
1H-isindole-1,3(2H)-dione, 2-[(trichloromethyl)thio]-	<chem>O=C(N(SCl)C(Cl)C(=O)c1cccc2)c12</chem>	2.85	2.84	-0.01	2.92	0.07
cyclohexanone, 2-methyl-5-(1-methylethenyl)-	<chem>O=C1CC(C(=C)C)CCC1C</chem>	2.85	2.86	0.01	2.39	-0.46
2-cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-	<chem>O=C(C=C(CC1)C)C1C(C)C</chem>	2.85	3.07	0.22	2.47	-0.38
benzoic acid, 4-bromo-	<chem>O=C(O)c(ccc(c1)Br)c1</chem>	2.86	2.76	-0.10	2.43	-0.43
cyclohexene	<chem>C=CCCCC1C</chem>	2.86	2.96	0.10	2.77	-0.09
1,5-hexadiene	<chem>C(=C)CCC=C</chem>	2.87	3.02	0.15	3.05	0.18
2-propenoic acid, 2-methyl-, butyl ester	<chem>O=C(OCCCC)C(=C)C</chem>	2.88	2.75	-0.13	2.59	-0.29
1,3(2H,9bH)-dibenzofurandione, 2,6-diacetyl-7,9-dihydroxy-8,9b-dimethyl-	<chem>O=C(c(c(OC(C1(C(=O)C(C2(=O))C(=O)C)C)=C2)c1c(O)c3C)c3O)C</chem>	2.88	2.78	-0.10	2.77	-0.11
pyridine, 4-[(4-nitrophenyl)methyl]-	<chem>N(=O)(=O)c(ccc(c1)Cc(ccnc2)c2)c1</chem>	2.88	2.88	0.00	2.74	-0.14
phenol, 2-(1-methylethyl)-	<chem>Oc(c(ccc1)C(C)C)c1</chem>	2.88	2.97	0.09	2.78	-0.10
3,5-pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, ethyl methyl ester	<chem>c1ccc(N(=O)=O)cc1C2C(C(=O)OC)=C(C)NC(C)=C2C(=O)OCC</chem>	2.88	2.99	0.11	3.21	-0.07
butane	<chem>C(C)C</chem>	2.89	2.31	-0.58	2.81	-0.08
propane, 2-iodo-	<chem>C(C)(C)I</chem>	2.89	2.50	-0.39	2.59	-0.30
9H-fluorene-9-methanol	<chem>OCC(c(c(c1cccc2)ccc3)c3)c12</chem>	2.89	2.69	-0.20	3.06	0.17
2-octanol	<chem>OC(CCCCCC)C</chem>	2.90	2.73	-0.17	2.96	0.06
1-octanamine	<chem>NCCCCCCCC</chem>	2.90	2.80	-0.10	3.24	0.34
phenol, 4-(1-methylethyl)-	<chem>Oc(ccc(c1)C(C)C)c1</chem>	2.90	2.97	0.07	2.84	-0.06
butane, 1-isothiocyanato-	<chem>N(=C=S)CCCC</chem>	2.92	2.77	-0.15	2.86	-0.06
benzene, (bromomethyl)-	<chem>BrCc(cccc1)c1</chem>	2.92	2.88	-0.04	2.76	-0.16
1H-indene	<chem>c(c(C=C1)ccc2)(c2)C1</chem>	2.92	3.25	0.33	3.04	0.12
azacyclotridecan-2-one	<chem>O=C(NCCCCCCCCCCC1)C1</chem>	2.92	3.61	0.69	3.41	0.49
phenol, 2-propyl-	<chem>Oc(c(ccc1)CCC)c1</chem>	2.93	3.04	0.11	2.95	0.02
benzene, ethenyl-	<chem>c(cccc1)(c1)C=C</chem>	2.95	2.89	-0.06	2.92	-0.03

benzene, 1,3-dimethyl-2-nitro-	<chem>N(=O)(=O)c(c(ccc1C)c1C</chem>	2.95	2.91	-0.04	2.76	-0.19
benzoic acid, 2-hydroxy-, ethyl ester	<chem>O=C(OCC)c(c(O)ccc1)c1</chem>	2.95	3.09	0.14	2.76	-0.19
1-naphthalenol, 5,6,7,8-tetrahydro-	<chem>c1c(O)c2CCCCc2cc1</chem>	2.95	3.48	0.53	2.83	-0.12
19-norpregn-4-en-20-yn-3-one, 17-hydroxy-, (17-alpha)-	<chem>CC34CCCC1C(CCC2=CC(=O)CCC12)C3CCC4(O)C#C</chem>	2.97	2.99	0.02	2.72	-0.25
7-oxabicyclo[2.2.1]heptane, 1-methyl-4-(1-methylethyl)-	<chem>O(C(Cc1)(CC2)C(C)C)C12C</chem>	2.97	3.13	0.16	2.31	-0.66
1,6-octadien-3-ol, 3,7-dimethyl-	<chem>OC(C=C)(CCC=C(C)C)C</chem>	2.97	3.38	0.41	2.68	-0.29
bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl-	<chem>O=CC(C(Cc1C2)C1(C)C)=C2</chem>	2.98	2.78	-0.20	3.03	0.05
ethanone, 1-[4-(1-methylethyl)phenyl]-	<chem>CC(=O)c1ccc(C(C)C)cc1</chem>	2.98	3.13	0.15	3.12	0.14
benzoic acid, 2-hydroxy-4-methyl-	<chem>Cc1ccc(C(=O)(O))c(O)c1</chem>	2.99	2.79	-0.20	2.39	-0.60
2-propenoic acid, 3-phenyl-, ethyl ester	<chem>O=C(OCC)C=Cc(cccc1)c1</chem>	2.99	2.85	-0.14	3.10	0.11
benzene, bromo-	<chem>c(cccc1)(c1)Br</chem>	2.99	2.88	-0.11	2.65	-0.34
cyclopentane	<chem>C(CCC1)C1</chem>	3.00	2.68	-0.32	2.88	-0.12
1-octanol	<chem>OCCCCCCCC</chem>	3.00	2.81	-0.19	3.21	0.21
urea, N,N-diphenyl-	<chem>O=C(Nc(cccc1)c1)Nc(cccc2)c2</chem>	3.00	2.97	-0.03	3.10	0.10
9,10-anthracenedione, 1,4-diamino-	<chem>O=C(c(c(C(=O)c1c(N)ccc2N)ccc3)c3)c12</chem>	3.00	3.16	0.16	3.00	0.00
benzoic acid, propyl ester	<chem>O=C(OCCC)c(cccc1)c1</chem>	3.01	2.81	-0.20	2.92	-0.09
4H-1-benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)-	<chem>Oc1cc(O)c2C(=O)C=C(c3ccc(O)cc3)Oc2c1</chem>	3.02	2.84	-0.18	3.07	0.05
benzoic acid, 4-iodo-	<chem>O=C(O)c(ccc(c1)I)c1</chem>	3.02	3.04	0.02	2.55	-0.47
phenol, 4,4-(3H-2,1-benzoxathiol-3-ylidene)bis-, S,S-dioxide	<chem>O=S(=O)(OC(c1cccc2)(c(ccc(O)c3)c3)c(ccc(O)c4)c4)c12</chem>	3.02	3.21	0.19	3.15	0.13
phenol, 2-methoxy-4-(1-propenyl)-	<chem>O(c(c(O)ccc1C=CC)c1)C</chem>	3.04	2.65	-0.39	2.79	-0.25
benzoic acid, 4-hydroxy-, propyl ester	<chem>O=C(OCCC)c(ccc(O)c1)c1</chem>	3.04	2.98	-0.06	3.28	0.24
cyclohexanone, 5-methyl-2-(1-methylethyl)-	<chem>O=C(C(CCC1C)C(C)C)C1</chem>	3.05	2.87	-0.18	2.65	-0.40
benzene, 1-bromo-4-methoxy-	<chem>O(c(ccc(c1)Br)c1)C</chem>	3.05	2.96	-0.09	2.93	-0.12
octanoic acid	<chem>O=C(O)CCCCCCC</chem>	3.05	3.03	-0.02	2.92	-0.13
benzenamine, 4-butyl-	<chem>Nc(ccc(c1)CCCC)c1</chem>	3.05	3.10	0.05	2.95	-0.10
2-naphthalenecarboxylic acid, 3-hydroxy-	<chem>O=C(O)c(c(O)cc(c1ccc2)c2)c1</chem>	3.05	3.42	0.37	3.30	0.25
1,3-benzenedicarbonitrile, 2,4,5,6-tetrachloro-erythromycin	<chem>N#Cc(c(c(c(c1C#N)Cl)Cl)Cl)c1Cl</chem>	3.05	3.66	0.61	3.98	0.93
	<chem>CCC3OC(=O)C(C)C(OC1CC(C)(OC)C(O)C(C)O1)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(C)(O)CC(C)C(=O)C(C)C(O)C3(C)O</chem>	3.06	2.48	-0.58	2.37	-0.69
2H-1,2-benzothiazine-3-carboxamide, 4-hydroxy-2-methyl-N-2-pyridinyl-, 1,1-dioxide	<chem>CN2C(=C(O)c1cccc1S2(=O)=O)C(=O)Nc3ccccc3</chem>	3.06	2.58	-0.48	2.20	-0.86
phenol, 2,5-dichloro-	<chem>Oc(c(ccc1Cl)Cl)c1</chem>	3.06	2.80	-0.26	3.13	0.07
phenol, 2,4-dichloro-	<chem>Oc(c(cc(c1)Cl)Cl)c1</chem>	3.06	2.80	-0.26	3.14	0.08
cyclohexanone, 5-methyl-2-(1-methylethylidene)-	<chem>O=C(C(=C(C)C)CCC1C)C1</chem>	3.08	3.20	0.12	2.36	-0.72
phenol, 4-(1-methylpropyl)-	<chem>Oc(ccc(c1)C(CC)C)c1</chem>	3.08	3.46	0.38	3.35	0.27
cholan-24-oic acid, 3,6-dihydroxy-, (3-alpha,5,6-alpha)-	<chem>O=C(CCC(C1C2(CCC3C4(C(C(CC3C2CC1)O)(CC(CC4)O))C)C)C(=O)C(O)C(c(cccc1)c1)c(cccc2)c2</chem>	3.08	5.06	1.98	2.98	-0.10
benzeneacetic acid, alpha-phenyl-[1,1-biphenyl]-2-ol	<chem>O=C(c(c(cccc1)c1)ccc2)c2</chem>	3.09	3.06	-0.03	2.79	-0.30
benzene, (2-bromoethyl)-	<chem>BrCCc(cccc1)c1</chem>	3.09	3.28	0.19	3.21	0.12
cyclohexanol, 4-(1,1-dimethylethyl)-	<chem>OC(CCC(C(C)C)C)C1C1</chem>	3.09	3.37	0.28	3.28	0.19
phenol, 4-chloro-3-methyl-	<chem>OC(c(c1C)Cl)c1</chem>	3.09	3.42	0.33	3.29	0.20
2,4-oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-	<chem>Oc(ccc(c1C)Cl)c1</chem>	3.10	2.70	-0.40	2.74	-0.36
propane, 2,2-dimethyl-	<chem>c1c(Cl)cc(Cl)cc1N2C(=O)C(C)(C=C)OC2(=O)</chem>	3.10	3.03	-0.07	2.81	-0.29
benzene, 1,2-dichloro-4,5-dimethoxy-	<chem>C(C)C(C)C</chem>	3.11	2.69	-0.42	2.95	-0.16
benzene, 1,2-dimethyl-	<chem>COc1c(OC)cc(Cl)c(Cl)c1</chem>	3.11	2.93	-0.18	3.34	0.23
benzene, 1,2-dichloro-4-nitro-	<chem>c(c(ccc1)C)(c1)C</chem>	3.12	3.09	-0.03	3.16	0.04
2-cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-	<chem>N(=O)(=O)c(ccc(c1Cl)Cl)c1</chem>	3.12	3.10	-0.02	3.11	-0.01
propanoic acid, 2-(4-chloro-2-methylphenoxy)-	<chem>C1(C)=CCC(C(C)=C)CC1O</chem>	3.12	3.29	0.17	2.41	-0.71
benzenemethanamine, N-phenyl-	<chem>O=C(O)C(Oc(c(cc(c1)Cl)C)c1)C</chem>	3.13	2.94	-0.19	2.87	-0.26
benzenamine, N-nitroso-N-phenyl-	<chem>N(c(cccc1)c1)Cc(cccc2)c2</chem>	3.13	3.03	-0.10	3.27	0.14
1-cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)-	<chem>O=NN(c(cccc1)c1)c(cccc2)c2</chem>	3.13	3.16	0.03	3.20	0.07
2-nonanone	<chem>O=CC(=CCC(C(=C)C)C1)C1</chem>	3.13	3.34	0.21	2.97	-0.16
benzene, ethyl-	<chem>O=C(CCCCCC)C</chem>	3.14	2.71	-0.43	3.08	-0.06
benzene, 1,4-dimethyl-	<chem>c(cccc1)(c1)CC</chem>	3.15	3.03	-0.12	3.27	0.12
bicyclo[3.1.1]hept-3-en-2-ol, 4,6,6-trimethyl-	<chem>c(ccc(c1)C)(c1)C</chem>	3.15	3.09	-0.06	3.15	0.00
ethane, 1,1,2-trichloro-1,2,2-trifluoro-	<chem>C1(C)C(C)C2C(O)C=C(C1C2)C</chem>	3.16	2.73	-0.43	2.07	-1.09
	<chem>FC(F)(C(F)(Cl)Cl)Cl</chem>	3.16	3.09	-0.07	3.03	-0.13

3,5-pyrazolidinedione, 4-butyl-1,2-diphenyl-	<chem>O=C(N(N(C(=O))c(cccc2)c2)c(cccc3)c3)C1CCCC</chem>	3.16	3.52	0.36	2.81	-0.35
1,5-cyclooctadiene	<chem>C(=CCCC=CC1)C1</chem>	3.16	3.73	0.57	3.58	0.42
bicyclo[2.2.1]heptan-2-ol, 1,3,3-trimethyl-	<chem>OC(C(C1C2)(C2)C)C1(C)C</chem>	3.17	2.85	-0.32	2.30	-0.87
1-cyclohexene-1-methanol, 4-(1-methylethenyl)-	<chem>OCC(=CCC(C(=C)C)C1)C1</chem>	3.17	3.36	0.19	2.50	-0.67
3-cyclohexene-1-ethanol, 4-methyl-methylene-	<chem>OCC(C(CCC(=C1)C)C1)=C</chem>	3.17	3.36	0.19	2.55	-0.62
benzoic acid, 1-methylethyl ester	<chem>O=C(OC(C)C)c(cccc1)c1</chem>	3.18	2.74	-0.44	2.72	-0.46
2-naphthaleneacetic acid, 6-methoxy-alpha-methyl-	<chem>COc2ccc1cc(ccc1c2)C(C)C(O)=O</chem>	3.18	3.10	-0.08	3.29	0.11
methanone, diphenyl-	<chem>O=C(c(cccc1)c1)c(cccc2)c2</chem>	3.18	3.15	-0.03	3.03	-0.15
pregna-1,4-diene-3,20-dione, 21-(acetyloxy)-6,9-	<chem>O=C1C=C2C(F)CC3C4CC5OC(C)</chem>	3.19	2.77	-0.42	2.93	-0.26
difluoro-11-hydroxy-16,17-[(1-methylethylidene)bis(oxy)]-, (6-alpha,11-beta,16-alpha)-	<chem>(C)OC5(C(=O)COC(=O)C)C4(C)CC(O)C3(F)C2(C)C=C1</chem>					
naphthalene, 1-nitro-	<chem>N(=O)(=O)c(c(c(ccc1)cc2)c1)c2</chem>	3.19	2.99	-0.20	3.20	0.01
cyclohexanol, 5-methyl-2-(1-methylethyl)-	<chem>OC(C(CCC1C)C(C)C)C1</chem>	3.19	3.38	0.19	2.68	-0.51
phenol, 4-propyl-	<chem>Oc(ccc(c1)CCC)c1</chem>	3.20	3.04	-0.16	3.01	-0.19
benzene, 1,3-dimethyl-	<chem>c(cccc1C)(c1)C</chem>	3.20	3.09	-0.11	3.15	-0.05
[1,1-biphenyl]-4-ol	<chem>Oc(ccc(c(cccc1)c1)c2)c2</chem>	3.20	3.28	0.08	3.24	0.04
azulene	<chem>C1=CC=C2C=CC=C2C=C1</chem>	3.20	3.38	0.18	3.51	0.31
7-oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-	<chem>O(C1(CCC(C(=C)C)C2)C)C12</chem>	3.20	3.43	0.23	2.81	-0.39
cyclohexane, bromo-	<chem>BrC(CCCCC1)C1</chem>	3.20	3.45	0.25	3.63	0.43
prost-13-en-1-oic acid, 11,15-dihydroxy-9-oxo-	<chem>CCCCCCC(O)C=CC1C(O)CC(=O)C1</chem>	3.20	3.73	0.53	3.04	-0.16
butane, 1,1-oxybis-	<chem>O(CCCC)CCCC</chem>	3.21	3.01	-0.20	3.04	-0.17
cyclohexanol, 2-methyl-5-(1-methylethenyl)-	<chem>OC(C(CCC1C(=C)C)C)C1</chem>	3.21	3.37	0.16	2.70	-0.51
bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	<chem>OCC(C(C1C2)C1(C)C)=C2</chem>	3.22	2.80	-0.42	2.71	-0.51
ethane, pentachloro-	<chem>C(C(Cl)Cl)(Cl)(Cl)Cl</chem>	3.22	3.11	-0.11	3.21	-0.01
androst-5-en-17-one, 3-hydroxy-, (3b)-	<chem>C1C(O)CC2=CCC3C4CCC(=O)C4(C)CCC3C2(C)C1</chem>	3.23	2.98	-0.25	3.53	0.30
[1,1-biphenyl]-3-ol	<chem>Oc(cccc1c(cccc2)c2)c1</chem>	3.23	3.28	0.05	3.19	-0.04
1,2-benzenedicarboxylic acid, di-2-propenyl ester	<chem>O=C(OCC=C)c(c(ccc1)C(=O)OCC=C)c1</chem>	3.23	3.36	0.13	2.71	-0.52
benzene, iodo-	<chem>c(cccc1)(c1)I</chem>	3.25	3.16	-0.09	3.00	-0.25
phenol, 4,5-dichloro-2-methoxy-	<chem>COc1cc(Cl)c(Cl)cc1O</chem>	3.26	2.63	-0.63	3.07	-0.19
3-cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-	<chem>OC(CCC(=C1)C)(C1)C(C)C</chem>	3.26	3.33	0.07	2.81	-0.45
butanoic acid, 3-methyl-, phenylmethyl ester	<chem>O=C(OCc(cccc1)c1)CC(C)C</chem>	3.26	3.48	0.22	3.35	0.09
ethanamine, 2-(diphenylmethoxy)-N,N-dimethyl-	<chem>CN(C)CCOC(c1ccccc1)c2ccccc2</chem>	3.27	3.11	-0.16	3.44	0.17
phenol, 4-chloro-3,5-dimethyl-	<chem>Oc(cc(c1C)Cl)C1</chem>	3.27	3.25	-0.02	3.14	-0.13
benzamide, 2-hydroxy-N-phenyl-	<chem>O=C(Nc(cccc1)c1)c(c(O)ccc2)c2</chem>	3.27	3.30	0.03	2.65	-0.62
phenol, 2-(1-methylpropyl)-	<chem>Oc(c(ccc1)C(CC)C)c1</chem>	3.27	3.46	0.19	3.14	-0.13
1,2-benzenedicarboxylic acid, dipropyl ester	<chem>O=C(OCCC)c(c(ccc1)C(=O)OCCC)c1</chem>	3.27	3.63	0.36	3.54	0.27
carbonic acid, diphenyl ester	<chem>O=C(OC(cccc1)c1)OC(cccc2)c2</chem>	3.28	3.21	-0.07	3.35	0.07
benzene, isothiocyanato-	<chem>N(c(cccc1)c1)=C=S</chem>	3.28	3.33	0.05	3.08	-0.20
terpineol	<chem>OC(C1CC=C(CC1)C)C(C)C</chem>	3.28	3.33	0.05	3.17	-0.11
thiocyanic acid, (2-benzothiazolylthio)methyl ester	<chem>c1ccc2N=C(SCS(C#N))Sc2c1</chem>	3.30	3.12	-0.18	3.29	-0.01
naphthalene	<chem>c(c(ccc1)ccc2)(c1)c2</chem>	3.30	3.17	-0.13	3.33	0.03
phenol, 5-methyl-2-(1-methylethyl)-	<chem>OC(c(ccc1C)C(C)C)c1</chem>	3.30	3.52	0.22	3.16	-0.14
benzenamine, N,N-diethyl-	<chem>N(c(cccc1)c1)(CC)CC</chem>	3.31	3.15	-0.16	3.43	0.12
phenol, 2-(1,1-dimethylethyl)-	<chem>OC(c(ccc1)C(C)C)C1</chem>	3.31	3.42	0.11	3.35	0.04
phenol, 4-(1,1-dimethylethyl)-	<chem>OC(ccc(c1)C(C)C)C1</chem>	3.31	3.42	0.11	3.47	0.16
benzene, 1,1-[oxybis(methylene)]bis-	<chem>O(Cc(cccc1)c1)Cc(cccc2)c2</chem>	3.31	3.48	0.17	3.42	0.11
androst-4-en-3-one, 17-hydroxy-, (17)-	<chem>C1C(=O)C=C2CCC3C4CCC(O)C4(C)CCC3C2(C)C1</chem>	3.32	3.27	-0.05	2.99	-0.33
phenol, 4,4-(1-methylethylidene)bis-	<chem>OC(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1</chem>	3.32	3.64	0.32	3.81	0.49
phenol, 4,4-thiobis-	<chem>OC(ccc(Sc(ccc(O)c1)c1)c2)c2</chem>	3.34	3.33	-0.01	3.73	0.39
propanamide, 2-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]-	<chem>c1c(C(F)F)c(N(=O)=O)ccc1NC(=O)C(C)C</chem>	3.35	3.51	0.16	2.55	-0.80
phenol, 4-phenoxy-	<chem>O(c(ccc(O)c1)c1)c(cccc2)c2</chem>	3.35	3.57	0.22	3.32	-0.03
cyclopentane, methyl-	<chem>C(CCC1)(C1)C</chem>	3.37	3.10	-0.27	3.15	-0.22
pentane, 1-bromo-	<chem>BrCCCCC</chem>	3.37	3.14	-0.23	3.27	-0.10
ethanedione, diphenyl-	<chem>O=C(c(cccc1)c1)C(=O)c(cccc2)c2</chem>	3.38	3.56	0.18	2.96	-0.42
pentane	<chem>C(CCC)C</chem>	3.39	2.80	-0.59	3.41	0.02
1-hexene	<chem>C(=C)CCCC</chem>	3.39	3.15	-0.24	3.38	-0.01
9,10-anthracenedione	<chem>O=C(c(c(C(=O)c1cccc2)ccc3)c3)c12</chem>	3.39	3.34	-0.05	2.83	-0.56
ethene, tetrachloro-	<chem>C(=C(Cl)Cl)(Cl)Cl</chem>	3.40	2.97	-0.43	3.13	-0.27

3-pyridinecarbonitrile, 5-[(4-chloro-2-nitrophenyl)azo]-1-ethyl-1,2-dihydro-6-hydroxy-4-methyl-2-oxo-	<chem>N(=O)</chem>	3.40	3.57	0.17	3.67	0.27
benzenamine, 4-(phenylazo)-	<chem>(=O)c1cc(Cl)ccc1N=NC2=C(O)N(CC)C(=O)C(C(=N))=C2C</chem>					
pyridine, 2-chloro-6-(trichloromethyl)-	<chem>N(=Nc(cccc1)c1)c(ccc(N)c2)c2</chem>	3.41	3.19	-0.22	4.02	0.61
2-piperidinecarboxamide, 1-butyl-N-(2,6-dimethylphenyl)-	<chem>n(c(ccc1)C(Cl)(Cl)Cl)c1Cl</chem>	3.41	3.35	-0.06	3.87	0.46
methane, tetrabromo-	<chem>N1(CCCC)C(C(=O)Nc2c(C)cccc2C)C</chem>	3.41	3.44	0.03	3.31	-0.10
butane, 2,3-dimethyl-	<chem>CCC1</chem>					
benzene, 1-chloro-2-methyl-	<chem>BrC(Br)(Br)Br</chem>	3.42	2.80	-0.62	3.30	-0.12
benzene, 1-bromo-4-methyl-	<chem>C(C(C)C)(C)C</chem>	3.42	3.14	-0.28	2.84	-0.58
nonanoic acid	<chem>c(c(ccc1)Cl)(c1)C</chem>	3.42	3.18	-0.24	3.27	-0.15
benzene, 1,3,5-trimethyl-	<chem>c(ccc(c1)Br)(c1)C</chem>	3.42	3.43	0.01	3.35	-0.07
benzene, 1,2-dichloro-	<chem>O=C(O)CCCCCCCC</chem>	3.42	3.52	0.10	3.47	0.05
cyclohexane	<chem>c(cc(cc1C)C)(c1)C</chem>	3.42	3.63	0.21	3.64	0.22
benzene, 1,4-dichloro-	<chem>c(c(ccc1)Cl)(c1)Cl</chem>	3.43	3.28	-0.15	3.45	0.02
cinchon-9-ol, 6-methoxy-	<chem>C(CCCC1)C1</chem>	3.44	3.18	-0.26	3.46	0.02
	<chem>c(ccc(c1)Cl)(c1)Cl</chem>	3.44	3.28	-0.16	3.46	0.02
	<chem>c12nccc(C(O)C3N4CCC(C(C=C)C4)C3)c1cc(OC)cc2</chem>	3.44	3.29	-0.15	2.82	-0.62
1,3-benzenediol, 4-hexyl-	<chem>Oc(c(ccc1O)CCCCC)c1</chem>	3.45	4.04	0.59	3.77	0.32
1-naphthalenamine, N,N-dimethyl-	<chem>N(c(c(c(ccc1)cc2)c1)c2)(C)C</chem>	3.46	3.35	-0.11	3.67	0.21
peroxide, dibenzoyl	<chem>O=C(OOC(=O)c(cccc1)c1)c(cccc2)c2</chem>	3.46	3.43	-0.03	2.75	-0.71
naphthalene, 2-methoxy-	<chem>O(c(ccc(c1ccc2)c2)c1)C</chem>	3.47	3.25	-0.22	3.37	-0.10
2,6-octadien-1-ol, 3,7-dimethyl-	<chem>OCC=C(CCC=C(C)C)C</chem>	3.47	3.47	0.00	2.89	-0.58
benzene, (2-isothiocyanatoethyl)-	<chem>N(=C=S)CCc(cccc1)c1</chem>	3.47	3.50	0.03	3.41	-0.06
benzene, (1-methylethenyl)-	<chem>c(C(=C)C)(ccccc1)c1</chem>	3.48	3.44	-0.04	3.31	-0.17
phenol, 2-methyl-5-(1-methylethyl)-	<chem>Oc(c(ccc1C(C)C)C)c1</chem>	3.49	3.52	0.03	3.20	-0.29
naphthalene, 1,2,3,4-tetrahydro-	<chem>c(c(ccc1)CCC2)(c1)C2</chem>	3.49	3.96	0.47	3.79	0.30
pregna-1,4-diene-3,20-dione, 21-chloro-9-fluoro-11-hydroxy-16-methyl-17-(1-oxopropoxy)-, (11-beta,16-beta)-	<chem>O=C1C=C2CCC3C4CC(C)C(OC(=O)CC)(C(=O)CCl)C4(C)CC(O)C3(F)C2(C)C=C1</chem>	3.50	2.98	-0.52	3.49	-0.01
9,10-anthracenedione, 1,4-diamino-2-methoxy-	<chem>O=C(c(c(C(=O)c1c(N)cc(OC)c2N)ccc3)c3)c12</chem>	3.50	3.24	-0.26	2.82	-0.68
benzenamine, N-phenyl-	<chem>N(c(cccc1)c1)c(cccc2)c2</chem>	3.50	3.29	-0.21	3.34	-0.16
cholan-24-oic acid, 3,12-dihydroxy-, (3-alpha,5,12-alpha)-	<chem>O=C(O)CCC(C(C(C(C(C(C1)CC(O)C2)(C2)C)C3)C1)C4)(C3O)C)C4)C</chem>	3.50	5.06	1.56	3.30	-0.20
3-pyridinecarboxylic acid, hexyl ester	<chem>n1cc(C(=O)OCCCCC)ccc1</chem>	3.51	3.10	-0.41	3.06	-0.45
bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-	<chem>O=C(C(CC1C2)(C2)C)C1(C)C</chem>	3.52	3.04	-0.48	2.54	-0.98
10H-phenothiazine-2-carbonitrile, 10-[3-(4-hydroxy-1-piperidinyl)propyl]-	<chem>c1ccc2Sc3ccc(C(=N))cc3N(CCCN4C(CO)CC4)c2c1</chem>	3.52	3.93	0.41	3.78	0.26
benzene, 1,3-dichloro-	<chem>c(cccc1Cl)(c1)Cl</chem>	3.53	3.28	-0.25	3.45	-0.08
benzene, 1-ethyl-2-methyl-	<chem>c(c(ccc1)C)(c1)CC</chem>	3.53	3.58	0.05	3.87	0.34
phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester	<chem>COP(=O)</chem>	3.53	3.81	0.28	3.93	0.40
phenol, 2-(1-methylpropyl)-4,6-dinitro-	<chem>(OC)OC(=CCl)c1cc(Cl)c(Cl)cc1Cl</chem>					
	<chem>N(=O)(=O)c(cc(N(=O)=O)(=O))c(O)c1C(CC)C)c1</chem>	3.56	3.67	0.11	3.37	-0.19
benzoic acid, 4-hydroxy-, phenylmethyl ester	<chem>O=C(OCc(cccc1)c1)c(ccc(O)c2)c2</chem>	3.56	3.70	0.14	3.66	0.10
2,5-pyridinedicarboxylic acid, dipropyl ester	<chem>n1cc(C(=O)OCCC)ccc1C(=O)OCCC</chem>	3.57	2.12	-1.45	2.61	-0.96
benzoic acid, 4-hydroxy-, butyl ester	<chem>O=C(OCCCC)c(ccc(O)c1)c1</chem>	3.57	3.47	-0.10	3.81	0.24
1,2-benzenediol, 3,4,6-trichloro-	<chem>Oc1c(Cl)cc(Cl)c(Cl)c1O</chem>	3.60	2.97	-0.63	3.55	-0.05
pentane, 3-methyl-	<chem>C(CC)(CC)C</chem>	3.60	3.21	-0.39	3.98	0.38
pregna-1,4-diene-3,20-dione, 9-fluoro-11,21-dihydroxy-16-methyl-17-[(1-oxopentyl)oxy]-, (11-beta,16-beta)-	<chem>C1=CC(=O)C=C2CCC3C4CC(C)C(O)C(=O)CCCC(C(=O)CO)C4(C)CC(O)C3(F)C12C</chem>	3.60	3.94	0.34	3.76	0.16
cyclohexane, methyl-	<chem>C(CCCC1)(C1)C</chem>	3.61	3.59	-0.02	3.90	0.29
benzene, ethylmethyl-	<chem>Cc1ccc(cc1)CC</chem>	3.63	3.58	-0.05	3.83	0.20
benzene, 1,2,4-trimethyl-	<chem>c(ccc(c1C)C)(c1)C</chem>	3.63	3.63	0.00	3.62	-0.01
ethanol, 2-(octylthio)-	<chem>OCCSCCCCCCCC</chem>	3.64	3.38	-0.26	3.88	0.24
benzene, 1,2-dibromo-	<chem>c(c(ccc1)Br)(c1)Br</chem>	3.64	3.77	0.13	3.77	0.13
phenol, 4-butyl-	<chem>Oc(ccc(c1)CCCC)c1</chem>	3.65	3.53	-0.12	3.55	-0.10
2-propanol, 1,3-dichloro-, phosphate (3:1)	<chem>O=P(OC(CCl)CCl)(OC(CCl)CCl)OC(CCl)CCl</chem>	3.65	3.65	0.00	3.26	-0.39
benzene, (1-methylethyl)-	<chem>c(cccc1)(c1)C(C)C</chem>	3.66	3.45	-0.21	3.67	0.01
benzene, 1,2,3-trimethyl-	<chem>c(c(c(cc1)C)C)(c1)C</chem>	3.66	3.63	-0.03	3.63	-0.03
9(10H)-anthracenone	<chem>O=C(c(c(ccc1)Cc2cccc3c1)c23</chem>	3.66	3.81	0.15	3.57	-0.09
benzenemethanol, alpha,alpha-diphenyl-	<chem>OC(c(cccc1)c1)</chem>	3.68	4.38	0.70	4.31	0.63

benzene, propyl-	(c(cccc2)c2)c(cccc3)c3					
methanesulfenamide, 1,1-dichloro-N-	c(cccc1)(c1)CCC	3.69	3.52	-0.17	3.86	0.17
[(dimethylamino)sulfonyl]-1-fluoro-N-phenyl-	CN(C)S(=O)(=O)N(SC(F)	3.70	2.72	-0.98	3.55	-0.15
4,7-methano-1H-isoindole-1,3(2H)-dione, 2-(2-	(Cl)Cl)c1cccc1					
ethylhexyl)-3a,4,7,7a-tetrahydro-	CCCCC(CC)CN3C(=O)C2C1CC(C(=	3.70	3.76	0.06	3.78	0.08
benzoic acid, 5-[2-chloro-4-	C1)C2C3(=O)					
(trifluoromethyl)phenoxy]-2-nitro-	O=C(O)c(c(N(=O)	3.70	4.17	0.47	3.87	0.17
	(=O))ccc1Oc(cc(c2)C(F)					
1,2-benzenediol, 3,4,5-trichloro-	(F)F)Cl)c2)c1					
cyclohexanamine, N-cyclohexyl-N-methyl-	c1(O)c(O)c(Cl)c(Cl)c(Cl)c1	3.71	2.97	-0.74	3.53	-0.18
3H-indol-3-one, 2-(1,3-dihydro-3-oxo-2H-indol-2-	N(C(CCCC1)C1)(C(CCCC2)C2)C	3.71	4.58	0.87	4.85	1.14
ylidene)-1,2-dihydro-	O=C(c(c(N1)ccc2)c2)C1=C(Nc(c3ccc	3.72	3.11	-0.61	2.76	-0.96
9H-carbazole	4)c4)C3(=O)					
phenol, 2,3,4-trichloro-6-methoxy-	n(c(c(c1cccc2)ccc3)c3)c12	3.72	3.23	-0.49	3.69	-0.03
cyclohexane, 1,2,3,4,5,6-hexachloro-,	COc1cc(Cl)c(Cl)c(Cl)c1O	3.72	3.27	-0.45	3.81	0.09
(1a,2a,3b,4a,5a,6b)-	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	3.72	4.26	0.54	3.94	0.22
phenol, 3,4,5-trichloro-2,6-dimethoxy-						
9,10-anthracenedione, 1-amino-	Oc1c(OC)c(Cl)c(Cl)c(Cl)c1OC	3.74	3.10	-0.64	3.81	0.07
	O=C(c(c(c(N)cc1)C(=O)c2cccc3)c1)c	3.74	3.53	-0.21	3.21	-0.53
	23					
benzenamine, 4-nitro-N-phenyl-	N(=O)(=O)c(ccc(Nc(cccc1)c1)c2)c2	3.74	3.69	-0.05	3.62	-0.12
propanedioic acid, 1,3-dithiol-2-ylidene-, bis(1-	S1C=CSC1=C(C(=O)OC(C)C)C(=O)	3.75	2.57	-1.18	3.58	-0.17
methylethyl) ester	OC(C)C					
ethanol, 2-butoxy-, phosphate (3:1)	O=P(OCCOCCCC)	3.75	3.00	-0.75	3.31	-0.44
	(OCCOCCCC)OCCOCCCC					
2,2-bithiophene	S1C=CC=C1C2=CC=CS2	3.75	3.40	-0.35	4.06	0.31
pregna-1,4-diene-3,11,20-trione, 21-chloro-9-fluoro-	O=C1C=C2CCC3C4CC(C)C(OC(=O)	3.76	3.67	-0.09	3.77	0.01
16-methyl-17-(1-oxobutoxy)-, (16-beta)-	CCC)					
	(C(=O)CCl)C4(C)CC(=O)C3(F)C2(C)					
	C=C1					
phenol, 3,4,5-trichloro-2-methoxy-	COc1c(O)cc(Cl)c(Cl)c1Cl	3.77	3.27	-0.50	3.81	0.04
1-nonanol	CCCCCCCCCCC	3.77	3.30	-0.47	3.76	-0.01
ethanamine, N,N-dimethyl-2-[(2-	O(C(c(cccc1)c1)c(c(ccc2)C)c2)CCN(	3.77	3.65	-0.12	3.50	-0.27
methylphenyl)phenylmethoxy]-	C)C					
methanone, (2-hydroxy-4-methoxyphenyl)phenyl-	O=C(c(cccc1)c1)c(c(O)cc(OC)c2)c2	3.79	3.52	-0.27	3.35	-0.44
phenol, 2,6-bis(1-methylethyl)-	Oc(c(ccc1)C(C)C)c1C(C)C	3.79	3.57	-0.22	3.81	0.02
benzene, 1,4-dibromo-	c(ccc(c1)Br)(c1)Br	3.79	3.77	-0.02	3.71	-0.08
benzoic acid, 2-hydroxy-, propyl ester	O=C(OCC)C(c(O)ccc1)c1	3.80	3.59	-0.21	3.19	-0.61
hexane, 1-bromo-	BrCCCCC	3.80	3.63	-0.17	3.88	0.08
phosphorothioic acid, o,o-diethyl o-[6-methyl-2-(1-	O(P(OCC)	3.81	3.86	0.05	4.45	0.64
methylethyl)-4-pyrimidinyl] ester	(Oc(nc(nc1C)C(C)C)c1)=S)CC					
butane, 2,2-dimethyl-	C(CC)(C)(C)C	3.82	3.18	-0.64	3.74	-0.08
diazene, diphenyl-	N(=Nc(cccc1)c1)c(cccc2)c2	3.82	4.11	0.29	4.30	0.48
6-octenal, 3,7-dimethyl-	O=CCC(CCC=C(C)C)C	3.83	3.53	-0.30	3.25	-0.58
benzoic acid, butyl ester	O=C(OCCCC)c(cccc1)c1	3.84	3.30	-0.54	3.40	-0.44
3-buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-	O=C(C=CC(=C(CCC1)C)C1(C)C)C	3.84	4.42	0.58	4.11	0.27
yl)-						
benzoic acid, 4-(1,1-dimethylethyl)-	O=C(O)c(ccc(c1)C(C)(C)C)c1	3.85	3.78	-0.07	3.32	-0.53
3-buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-	O=C(C=CC(C(=CCC1)C)C1(C)C)C	3.85	4.29	0.44	4.14	0.29
yl)-, (E)-						
pregna-1,4-diene-3,20-dione, 21-(2,2-dimethyl-1-	O=C1C=C2C(F)CC3C4CC(C)C(O)	3.86	3.69	-0.17	3.21	-0.65
oxopropoxy)-6,9-difluoro-11,17-dihydroxy-16-	(C(=O)COC(=O)C(C)					
methyl-, (6-alpha,11-beta,16-alpha)-	(C)C)C4(C)CC(O)C3(F)C2(C)C=C1					
naphthalene, 2-methyl-	c(c(ccc1C)ccc2)(c2)c1	3.86	3.72	-0.14	3.83	-0.03
10-undecenoic acid	O=C(O)CCCCCCCCC=C	3.86	4.37	0.51	3.84	-0.02
methanone, bis[4-(dimethylamino)phenyl]-	O=C(c(ccc(N(C)C)c1)c1)c(ccc(N(C)C)	3.87	3.50	-0.37	3.74	-0.13
	)c2)c2					
naphthalene, 1-methyl-	c(c(c(cc1)C)ccc2)(c2)c1	3.87	3.72	-0.15	3.84	-0.03
thioperoxydicarbonic diamide, tetraethyl-	N(C(=S)SSC(N(CC)CC)=S)(CC)CC	3.88	3.67	-0.21	3.88	0.00
methanesulfenamide, 1,1-dichloro-N-	CN(C)S(=O)(=O)N(SC(F)	3.90	3.27	-0.63	3.90	0.00
[(dimethylamino)sulfonyl]-1-fluoro-N-(4-	(Cl)Cl)c1ccc(C)cc1					
methylphenyl)-						
hexane	C(CCCC)C	3.90	3.29	-0.61	4.02	0.12
naphthalene, 1-chloro-	c(c(c(cc1)Cl)ccc2)(c2)c1	3.90	3.81	-0.09	3.95	0.05
benzenamine, 4,4'-methylenebis[2-chloro-]	Nc(c(cc(c1)Cc(ccc(N)c2Cl)c2)Cl)c1	3.91	3.47	-0.44	3.72	-0.19
6-octen-1-ol, 3,7-dimethyl-	CCCC(CCC=C(C)C)C	3.91	3.56	-0.35	3.48	-0.43
acenaphthylene, 1,2-dihydro-	c(c(ccc1)ccc2)(c1CC3)c23	3.92	4.15	0.23	4.01	0.09

phenol, 4-chloro-5-methyl-2-(1-methylethyl)-	<chem>Oc(c(cc(c1C)Cl)C(C)C)c1</chem>	3.92	4.16	0.24	3.75	-0.17
cyclohexene, 4-ethenyl-	<chem>C(=CCCC1C=C)C1</chem>	3.93	3.73	-0.20	3.49	-0.44
1,6-octadien-3-ol, 3,7-dimethyl-, acetate	<chem>O=C(OC(C=C)(CCC=C(C)C)C)C</chem>	3.93	4.39	0.46	4.03	0.10
propanamide, N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-, 2-hydroxy-	<chem>O=C(N(C2(CCN(C2)CCc3cccs3)COC)c1ccccc1)CC</chem>	3.95	3.62	-0.33	3.40	-0.55
1,2,3-propanetricarboxylate (1:1)	<chem>c(ccc(c1Cl)Cl)(c1)C</chem>	3.95	3.83	-0.12	3.97	0.02
benzene, 1,2-dichloro-4-methyl-	<chem>O=C(OC(C1CC=C(C(C1)C)(C)C)C</chem>	3.96	4.34	0.38	4.32	0.36
terpineol, acetate	<chem>O=C(OCc(cccc1)c1)c(cccc2)c2</chem>	3.97	3.54	-0.43	3.43	-0.54
benzoic acid, phenylmethyl ester	<chem>O=C(O)C(c(ccc(c1)CC(C)C)c1)C</chem>	3.97	3.79	-0.18	3.50	-0.47
benzeneacetic acid, alpha-methyl-4-(2-methylpropyl)-	<chem>c(ccc(c1C)Cl)(c1)Cl</chem>	3.97	3.83	-0.14	3.97	0.00
benzene, 1,4-dichloro-2-methyl-	<chem>c(c(cccc1)c1)(cccc2)c2</chem>	3.98	3.76	-0.22	4.02	0.04
1,1-biphenyl	<chem>c(c(ccc1Cl)ccc2)(c2)c1</chem>	3.98	3.81	-0.17	3.91	-0.07
naphthalene, 2-chloro-	<chem>O=C(OC=C(CCC=C(C)C)C)C</chem>	3.98	4.48	0.50	4.11	0.13
2,6-octadien-1-ol, 3,7-dimethyl-, acetate	<chem>C(=C)CCCCC</chem>	3.99	3.64	-0.35	4.00	0.01
1-heptene	<chem>O=P(OCCCC)(OCCCC)OCCCC</chem>	4.00	3.82	-0.18	3.65	-0.35
phosphoric acid tributyl ester	<chem>N(=O)</chem>	4.00	3.87	-0.13	4.45	0.45
propanenitrile, 3-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl](2-hydroxyethyl)amino]-	<chem>(=O)c(ccc(N=Nc(ccc(N(CCC(#N))CCO)c1)c1)c2Cl)c2</chem>					
benzene, 1,2,4,5-tetramethyl-	<chem>c(c(cc(c1C)C)C)(c1)C</chem>	4.00	4.18	0.18	4.05	0.05
benzene, 1,2,3,4-tetramethyl-	<chem>c(c(c(c1C)C)C)(c1)C</chem>	4.00	4.18	0.18	4.07	0.07
cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate	<chem>CC1CCCC(C)C(C)C(C1)OC(=O)C</chem>	4.00	4.39	0.39	3.54	-0.46
benzene, 1,2,3-trichloro-4,5-dimethoxy-	<chem>COc1c(OC)c(Cl)c(Cl)c(Cl)c1</chem>	4.01	3.57	-0.44	3.94	-0.07
estra-1,3,5(10)-triene-3,17-diol (17-beta)-	<chem>CC34CCC1C(CC2cc(O)ccc12)C3CC4O</chem>	4.01	3.94	-0.07	3.57	-0.44
benzoic acid, 2-phenylethyl ester	<chem>O=C(OCc(cccc1)c1)c(cccc2)c2</chem>	4.01	4.03	0.02	3.86	-0.15
benzene, 1,2,4-trichloro-	<chem>c(ccc(c1Cl)Cl)(c1)Cl</chem>	4.02	3.93	-0.09	4.08	0.06
benzene, 1,2,3-trichloro-	<chem>c(c(c(cc1Cl)Cl)(c1)Cl</chem>	4.05	3.93	-0.12	4.07	0.02
pregna-1,4-diene-3,20-dione, 9-fluoro-11-hydroxy-16-methyl-17,21-bis(1-oxopropoxy)-, (11-beta,16-beta)-	<chem>C1=CC(=O)C=C2CCC3C4CC(C)C(O C(=O)CC)(C(=O)COC(=O)CC)C4(C)CC(O)C3(F)C12C</chem>	4.07	3.66	-0.41	3.38	-0.69
propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(6-nitro-2-benzothiazolyl)azo]phenyl]amino]-	<chem>N1c2ccc(N(=O)(=O))cc2SC=1N=Nc3ccc(N(CCC(#N)CCOC(=O)C)cc3</chem>	4.08	3.83	-0.25	4.63	0.55
2-undecanone	<chem>O=C(CCCCCCCCCC)C</chem>	4.09	3.69	-0.40	4.25	0.16
decanoic acid	<chem>CCCCCCCCCCC(=O)O</chem>	4.09	4.02	-0.07	3.93	-0.16
benzene, methyl(1-methylethyl)-	<chem>Cc1ccc(C(C)C)cc1</chem>	4.10	4.00	-0.10	4.17	0.07
9,10-anthracenedione, 1-(methylamino)-	<chem>O=C(c(c(c(NC)cc1)C(=O)c2ccccc3)c1)c23</chem>	4.10	4.07	-0.03	3.02	-1.08
benzene, 1,2,3,5-tetramethyl-	<chem>c(cc(c(c1C)C)C)(c1)C</chem>	4.10	4.18	0.08	4.06	-0.04
[1]benzopyrano[3,4-b]furo[2,3-H][1]benzopyran-6(6aH)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-	<chem>COc5cc4OCC3Oc2c1CC(Oc1ccc2C(=O)C3c4cc5OC)C(C)=C</chem>	4.10	4.31	0.21	2.30	-1.80
benzene, (1,1-dimethylethyl)-	<chem>c(cccc1)(c1)C(C)(C)C</chem>	4.11	3.90	-0.21	4.49	0.38
1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester	<chem>O=C(OC(C)C)c(c(ccc1)C(=O)OCC(C)C)c1</chem>	4.11	4.46	0.35	3.98	-0.13
dibenzofuran	<chem>o(c(c(c1cccc2)ccc3)c3)c12</chem>	4.12	3.71	-0.41	3.92	-0.20
phenol, 2,4,6-tribromo-	<chem>Oc(c(cc(c1)Br)Br)c1Br</chem>	4.13	4.18	0.05	4.20	0.07
benzene, 1,1-methylenebis-	<chem>c(cccc1)(c1)Cc(cccc2)c2</chem>	4.14	4.02	-0.12	4.33	0.19
ethane, hexachloro-	<chem>C(C(Cl)(Cl)Cl)(Cl)(Cl)Cl</chem>	4.14	4.03	-0.11	3.93	-0.21
1-butanol, 3-methyl-, benzoate	<chem>O=C(OC(C)C)c(cccc1)c1</chem>	4.15	3.72	-0.43	3.59	-0.56
10H-phenothiazine	<chem>N(c(c(Sc1cccc2)ccc3)c3)c12</chem>	4.15	3.82	-0.33	4.19	0.04
cholan-24-oic acid, 3,7-dihydroxy-, (3-alpha,5,7-alpha)-	<chem>CC(CCC(=O)(O))C3CCC4C2C(O)CC1CC(O)CCC1(C)C2CCC34C</chem>	4.15	5.06	0.91	3.01	-1.14
(-)-flurbiprofen	<chem>OC(=O)C(C)C1cc(F)c(c2ccccc2)cc1</chem>	4.16	3.81	-0.35	3.57	-0.59
bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-	<chem>C(C(C1C2)C1(C)C)(C2)=C</chem>	4.16	4.35	0.19	3.94	-0.22
1,3,7-octatriene, 3,7-dimethyl-	<chem>C(CCC=C(C=C)C)(=C)C</chem>	4.17	4.88	0.71	4.25	0.08
1,6-octadiene, 7-methyl-3-methylene-	<chem>C(C=C)(=C)CCC=C(C)C</chem>	4.17	4.88	0.71	4.32	0.15
9H-fluorene	<chem>c(c(c(c1ccc2)c2)ccc3)(c3)C1</chem>	4.18	4.02	-0.16	4.26	0.08
benzene, ethenylethyl-	<chem>C=Cc1ccc(cc1)CC</chem>	4.19	3.93	-0.26	3.98	-0.21
benzene, 1,3,5-trichloro-	<chem>c(cc(cc1Cl)Cl)(c1)Cl</chem>	4.19	3.93	-0.26	4.08	-0.11
1-piperazineethanol, 4-[3-(2-chloro-10H-phenothiazin-10yl)propyl]-	<chem>OCCN4CCN(CCCN2c1ccccc1Sc3cc c(Cl)cc23)CC4</chem>	4.20	3.82	-0.38	4.15	-0.05
1-naphthalenamine, N-phenyl-	<chem>N(c(c(c(ccc1)cc2)c1)c2)c(cccc3)c3</chem>	4.20	4.47	0.27	4.57	0.37

diphenyl oxide	O(c(cccc1)c1)c(cccc2)c2	4.21	4.05	-0.16	3.68	-0.53
phenol, 4-cyclohexyl-	Oc(ccc(c1)C(CCCC2)C2)c1	4.22	4.33	0.11	4.38	0.16
bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-	C(C(C(C1C2)C2)(C1(C)C)=C	4.22	4.35	0.13	4.56	0.34
benzene, 2,4-dichloro-1-methyl-	c(ccc(c1Cl)C)(c1)Cl	4.24	3.83	-0.41	3.95	-0.29
1,3-cyclohexadiene, 1-methyl-4-(1-methylethyl)-	C(=CC=C(C1)C)(C1)C(C)C	4.25	4.75	0.50	4.51	0.26
1-piperidinepropanol, alpha-bicyclo[2.2.1]hept-5-en-2-yl-alpha-phenyl-	OC(c(cccc1)c1) (C(C(C=CC23)C2)C3)CCN(CCCCC4) C4	4.25	4.95	0.70	4.28	0.03
phenol, 2,2'-methylenebis[4-chloro-]	Oc(c(cc(c1)Cl)Cc(c(O)ccc2Cl)c2)c1	4.26	4.34	0.08	3.93	-0.33
phosphoric acid, dibutyl phenyl ester	O=P(OCCCC)(OCCCC)Oc(cccc1)c1	4.27	4.11	-0.16	3.74	-0.53
1H-indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-	COc1ccc2n(C(=O)c3ccc(Cl)cc3)c(C) c(CC(=O)O)c2c1	4.27	4.23	-0.04	4.25	-0.02
1,2-benzenediol, 3,4,5,6-tetrachloro-	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1O	4.29	3.61	-0.68	4.26	-0.03
1-propanamine, 3-dibenz[b,e]oxepin-11(6H)-ylidene-N,N-dimethyl-	CN(C)CCC=C2c1cccc1COc3cccc2 3	4.29	3.99	-0.30	4.08	-0.21
1-butanone, 4-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)-	OC2(CCN(CCCC(=O)c1ccc(F)cc1)C C2)c3ccc(Cl)cc3	4.30	4.20	-0.10	3.70	-0.60
ethanol, 2-[ethyl[4-[(4-nitrophenyl)azo]phenyl]amino]-	N(=O) (=O)c(ccc(N=Nc(ccc(N(CCO)CC)c1)c 1)c2)c2	4.30	4.20	-0.10	4.29	-0.01
ethanol, 2,2'-[[4-[(2-chloro-4-nitrophenyl)azo]-3-methylphenyl]imino]bis-	N(=O) (=O)c(ccc(N=Nc(cc(N(CCO)CCO)c 1)C)c1)c2Cl)c2	4.30	4.33	0.03	3.74	-0.56
cyclopropanecarboxylic acid, 3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-2,2-dimethyl-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester	O=C(OC(C(=C(C1(=O))CC=CC=C)C)C1)C(C2(C)C)C2C=C(C(=O)OC)C	4.30	5.33	1.03	4.25	-0.05
phenol, 2-(2H-benzotriazol-2-yl)-4-methyl-2,2-biquinoline	Oc1ccc(C)cc1n2nc3cccc3n2 n(c(c(ccc1)cc2)c1)c2c(nc(c(ccc3)c4)c 3)c4	4.31	3.00	-1.31	2.64	-1.67
piperazine, 1-acetyl-4-[4-[(2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl)methoxy]phenyl]-	CC(=O)N(C1)CCN(C1)c(c2)ccc(c2)O CC(CO3)OC3(Cn4cncc4)c5c(Cl)cc(C l)cc5	4.31	4.06	-0.25	4.31	0.00
heptane, 1-bromo-	BrCCCCCCCC	4.35	4.45	0.10	4.30	-0.05
benzoic acid, 2-(phenylamino)-	O=C(O)c(c(Nc(cccc1)c1)ccc2)c2	4.36	4.12	-0.24	4.40	0.04
9,10-anthracenedione, 2-ethyl-	O=C(c(c(C(=O)c1cccc2)ccc3CC)c3)c 12	4.36	4.18	-0.18	4.19	-0.17
2-cyclohexen-1-one, 2-[1-(ethoxyimino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxy-	CCCC(=NOCC)C1=C(O)CC(CC(C)S CC)CC1(=O)	4.37	4.38	0.01	3.69	-0.68
benzene, butyl-	c(cccc1)(c1)CCCC	4.38	3.99	-0.39	3.89	-0.49
dibenzothiophene	s(c(c(c1cccc2)ccc3)c3)c12	4.38	4.01	-0.37	4.34	-0.04
2-naphthalenamine, N-phenyl-	N(c(ccc(c1ccc2)c2)c1)c(cccc3)c3	4.38	4.17	-0.21	4.38	0.00
bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-	C(=CCC(C12)C1(C)C)(C2)C	4.38	4.47	0.09	4.53	0.15
3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile, 4-ethoxy-7-phenyl-, 4-sulfide	CCOP(=S) (OCC)ON=C(C(#N))c1ccccc1	4.38	4.61	0.23	3.64	-0.74
2-propenoic acid, 2-methyl-, 2-ethyl-2-[[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester	O=C(OCC(CC) (COC(=O)C(=C)C)COC(=O)C(=C)C) C(=C)C	4.39	4.39	0.00	3.78	-0.61
4-quinolinecarboxamide, 2-butoxy-N-[2-(diethylamino)ethyl]-	CCCCOc2cc(C(=O)NCCN(CC)CC)c1 ccccc1n2	4.39	4.50	0.11	3.00	-1.39
decanoic acid, methyl ester	O=C(OC)CCCCCCCCC	4.40	4.04	-0.36	3.79	-0.61
disulfide, diphenyl	S(Sc(ccc1)c1)c(cccc2)c2	4.41	4.30	-0.11	4.58	0.17
2,5-cyclohexadiene-1,4-dione, 2,5-bis(1,1-dimethylethyl)-	O=C1C(C(C) (C)C)=CC(=O)C=C1C(C)(C)C	4.41	4.31	-0.10	4.51	0.10
undecanoic acid	O=C(O)CCCCCCCCC	4.42	4.07	-0.35	3.79	-0.63
[1,1-biphenyl]-3-carboxylic acid, 2,4-difluoro-4-hydroxy-	c1c(C(=O)O)c(O)ccc1c2c(F)cc(F)cc2	4.42	4.51	0.09	4.49	0.07
bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-	C(=CC(C1C2)C1(C)C)(C2)C	4.44	4.41	-0.03	3.11	-1.33
phenol, 2,3,4,6-tetrachloro-	Oc(c(cc(c1Cl)Cl)Cl)c1Cl	4.44	4.61	0.17	3.26	-1.18
benzene, 1,1-thiobis-	S(c(cccc1)c1)c(cccc2)c2	4.45	4.09	-0.36	4.37	-0.08
anthracene	c(c(ccc1)cc(c2ccc3)c3)(c1)c2	4.45	4.29	-0.16	4.36	-0.09
2-propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester	O=C(OC=Cc(cccc1)c1)C=Cc(cccc2) c2	4.45	4.35	-0.10	4.56	0.11
phenanthrene	O=C(OCC=Cc(cccc1)c1)C=Cc(cccc2) c2	4.45	4.83	0.38	4.62	0.17
cyclohexene, 1-methyl-4-(1-methylethylidene)-	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3	4.46	4.46	0.00	4.46	0.00
1-piperidinepropanol, alpha-cyclohexyl-alpha-phenyl-	C(=C(C)C)(CCC(=C1)C)C1	4.46	4.35	-0.11	4.55	0.09
1,2-benzenedicarboxylic acid, dibutyl ester	OC(c(cccc1)c1) (C(CCCC2)C2)CCN(CCCC3)C3	4.47	4.88	0.41	3.82	-0.65
	O=C(OCCCC)c(c(ccc1)C(=O)OCCC	4.49	5.27	0.78	4.93	0.44
		4.50	4.61	0.11	4.53	0.03

1,4-cyclohexadiene, 1-methyl-4-(1-methylethyl)-2-octene	C)c1 C(=CCC(=C1)C)(C1)C(C)C	4.50	4.75	0.25	4.36	-0.14
benzene, 1,3,5-tribromo-2-propenoic acid, 2-methyl-, 2-ethylhexyl ester	C(=CC)CCCCC c(cc(cc1Br)Br)(c1)Br	4.51	4.06	-0.45	4.59	0.08
1-pentene, 2,4,4-trimethyl-9,10-anthracenedione, 1,4-diamino-2,3-dichloro-	O=C(OCC(CCCC)CC)C(=C)C C(=C)(CC(C)(C)C)C	4.54	4.64	0.10	4.57	0.03
benzene, tetrachloro-1-decanol	O=C(c(c(C(=O)c1c(N)c(c(c2N)Cl)Cl)c cc3)c3)c12	4.56	4.45	-0.11	4.11	-0.45
benzene, (1-methylpropyl)-1-octene	Clc2c(cc(cc2Cl)Cl)Cl OCCCCCCCCC	4.56	4.57	0.01	4.63	0.07
cyclohexene, 1-methyl-4-(1-methylethenyl)-benzene, diethyl-	c(cccc1)(c1)C(CC)C C(=C)CCCCC	4.57	3.79	-0.78	4.24	-0.33
benzenamine, N,N-dimethyl-4-(phenylazo)-phenol, 2,3,4,5-tetrachloro-6-methoxy-	C(=CCC(C(=C)C)C1)(C1)C CCc1ccc(cc1)CC	4.57	4.13	-0.44	4.61	0.04
phosphoric acid, triphenyl ester	N(=Nc(cccc1)c1)c(ccc(N(C)C)c2)c2 COc1c(O)c(Cl)c(Cl)c(Cl)c1Cl	4.58	4.29	-0.29	4.63	0.05
benzenesulfonamide, 3-nitro-N-phenyl-4-(phenylamino)-	O=P(Oc(cccc1)c1) (Oc(cccc2)c2)Oc(cccc3)c3	4.59	3.92	-0.67	4.44	-0.15
benzene, 1,2,3,4-tetrachloro-dodecanoic acid	O=S(=O) (Nc(cccc1)c1)c(ccc(Nc(cccc2)c2)c3N (=O)(=O))c3	4.60	4.33	-0.27	3.79	-0.81
1,1-biphenyl, 4-methyl-1,4-pentanediamine, N,4-(7-chloro-4-quinolyl)-N,N-diethyl-, phosphate (1:2)	c(c(c(c(c1)Cl)Cl)Cl)(c1)Cl O=C(O)CCCCCCCCC	4.60	4.57	-0.03	4.62	0.02
benzene, 1,2,4,5-tetrachloro-2,6-methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-heptane	c1ccccc1c2ccc(C)cc2 c12nccc(NC(C)CCCN(CC)CC)c1ccc(Cl)c2	4.63	4.30	-0.33	4.42	-0.21
oxazole, 2,5-diphenyl-benzene, (2-methylpropyl)-10H-phenothiazine-10-propanamine, 2-methoxy-N,N-beta-trimethyl-	c(c(cc(c1Cl)Cl)Cl)(c1)Cl CC2C3Cc1ccc(O)cc1C2(C)CCN3CC	4.64	4.57	-0.07	4.61	-0.03
piperidine, 4-(5H-dibenzo[a,d]cyclohepten-5-ylidene)-1-methyl-13-oxabicyclo[10.1.0]tridecane	=C(C)C C(CCCC)C	4.64	5.03	0.39	4.44	-0.20
10H-phenothiazine-10-propanamine, N,N-beta-trimethyl-, 2,3-dihydroxybutanedioate (2:1)	o(c(c(cccc1)c1)cn2)c2c(cccc3)c3 c(cccc1)(c1)CC(C)C	4.66	3.78	-0.88	4.33	-0.33
cyclohexane, 1,2,3,4,5-pentabromo-6-chloro-1,2-benzenedicarboxylic acid, butyl phenylmethyl ester	c1ccc2Sc3ccc(OC)cc3N(CC(C)CN(C) C)c2c1	4.67	3.74	-0.93	4.03	-0.64
1,3-benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-phenol, 5-chloro-2-(2,4-dichlorophenoxy)-	N(CCC(=C(c(c(C=Cc1cccc2)ccc3)c3) c12)C4)(C4)C	4.68	3.94	-0.74	4.13	-0.55
10H-phenothiazine-10-ethanamine, N,N-alpha-trimethyl-	C1OC1CCCCCCCCC=C c12N(CC(C)CN(C)C)c3ccccc3Sc1cc cc2	4.68	5.06	0.38	4.84	0.16
1,3-butadiene, 1,1,2,3,4,4-hexachloro-cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl ester	BrC(C(C(Br)C(Br)C1Br)Cl)C1Br O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)O CCCC)c2	4.72	4.71	-0.01	4.00	-0.72
benzene, 1,1-(1,2-ethenediyl)bis-acetamide, N-[5-bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-	O(c(c(O1)cc(c2CCC)COCCOCCOC CCC)c2)C1	4.73	4.84	0.11	4.54	-0.19
10H-phenothiazine-10-ethanamine, N,N-alpha-trimethyl-	O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl) c2	4.75	4.29	-0.46	3.07	-1.68
benzene, 1,1-(1,2-ethenediyl)bis-bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-	c1cc2Sc3ccccc3N(CC(C)N(CC)CC)c 2cc1	4.76	4.66	-0.10	5.53	0.77
benzene, 1,2,3,4-tetrachloro-5,6-dimethoxy-10H-phenothiazine, 2-chloro-10-[3-(4-methyl-1-piperazinyl)propyl]-pyrene	C(=C(C(=C(Cl)Cl)Cl)Cl)(Cl)Cl O=C(OC(C(=C(C1(=O))CC=C(C)C)C1) C(C2(C)C)C2C=C(C)C	4.77	5.47	0.70	5.75	0.98
octane, 1-bromo-phenol, 2,6-bis(1,1-dimethylethyl)-1-propanamine, 3-(10,11-dihydro-5H-	c(cccc1)(c1)CCc(cccc2)c2 O=C(OCCN(c(c(OC)cc(N=Nc(c(cc(N(=O)(=O))c1)Br)c1N(=O) (=O))c2NC(=O)C)c2)CCOC(=O)C)C	4.78	4.72	-0.06	4.86	0.08
	c1ccc2Sc3ccccc3N(CC(C)N(C)C)c2c 1	4.78	5.52	0.74	3.58	-1.20
	c(cccc1)(c1)C=Cc(cccc2)c2 C(C(C(C1C2)C1(C)C)C)(=C2)C	4.81	4.49	-0.32	4.52	-0.29
	COc1c(Cl)c(Cl)c(Cl)c(Cl)c1OC CN4CCN(CCCN2c1ccccc1Sc3ccc(Cl))cc23)CC4	4.81	4.52	-0.29	4.58	-0.23
	c(c(c(cc1)ccc2)c2cc3)(c1ccc4)c34 BrCCCCCCCC	4.83	4.27	-0.56	3.66	-1.17
	Oc(c(ccc1)C(C)(C)C)c1C(C)(C)C CN(C)CCC=C2c1ccccc1CCc3ccccc2	4.86	4.22	-0.64	4.64	-0.22
		4.88	4.79	-0.09	4.67	-0.21
		4.88	4.93	0.05	5.19	0.31
		4.89	4.61	-0.28	4.91	0.02
		4.92	4.48	-0.44	4.90	-0.02
		4.92	4.95	0.03	5.10	0.18

dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1,1-biphenyl, 4-bromo-phosphorothioic acid, o,o-diethyl o-(3,5,6-trichloro-2-pyridinyl) ester	3	<chem>c(ccc(c(cccc1)c1)c2)(c2)Br</chem>	4.96	4.65	-0.31	4.57	-0.39
1H-indene-1,3(2H)-dione, 2-(3-hydroxy-2-quinolinyl)-decane		<chem>CCOP(=S)</chem>	4.96	4.66	-0.30	5.15	0.19
10H-phenothiazine, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)-1,3-cyclopentadiene, 1,2,3,4,5,5-hexachloro-anthracene, 9-methyl-benzene, 1,1'-(2,2,2-trichloroethylidene)bis[4-methoxy-]phenol, 2,6-bis(1,1-dimethylethyl)methyl-benzene, hexamethyl-phenol, pentachloro-benzoic acid, 2-[(2,3-dimethylphenyl)amino]-1-dodecanol		<chem>O=C(c(c(C1(=O))ccc2)c2)C1c(nc(c(cc3)c4)c3)c4O</chem>	5.00	4.83	-0.17	3.29	-1.71
benzene, 1-(1,1-dimethylethyl)-4-methyl-benzene, pentachloro-octane		<chem>C(CCCCCCCC)C</chem>	5.01	5.25	0.24	5.87	0.86
phenol, 2,4-bis(1,1-dimethylethyl)-9,10-anthracenedione, 1,4-diamino-2,3-diphenoxy-5H-dibenz[b,f]azepine-5-propanamine, 3-chloro-10,11-dihydro-N,N-dimethyl-1,1-biphenyl, (1-methylethyl)-benzene, 1,1',1''-(chloromethylidyne)tris-benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)-2-propenylamino]-4-methoxyphenyl]-10H-phenothiazine-10-propanamine, 2-chloro-N,N-dimethyl-dodecanoic acid, methyl ester		<chem>CN4CCN(CCCN2c1cccc1Sc3ccc(cc23)C(F)(F)F)CC4</chem>	5.03	5.11	0.08	4.87	-0.16
1,3-benzenedicarbonitrile, 2-[[4-[[2-(acetoxy)ethyl]butylamino]-2-methylphenyl]azo]-5-nitro-peroxide, bis(1-methyl-1-phenylethyl)-cyclohexane, 1-methyl-4-(1-methylethyl)-phenol, isononyl-1,2-benzenedicarboxylic acid, dipentyl ester		<chem>C(=C(C(=C1Cl)Cl)Cl)(C1(Cl)Cl)Cl</chem>	5.04	4.63	-0.41	4.85	-0.19
		<chem>c(c(c(c1ccc2)c2)C)ccc3)(c3)c1</chem>	5.07	4.89	-0.18	5.06	-0.01
		<chem>OCc1ccc(cc1)C(c2ccc(OC)cc2)C(Cl)(Cl)Cl</chem>	5.08	5.67	0.59	5.12	0.04
		<chem>CC(c1cc(cc(c1O)C(C)(C)C)C(C)C</chem>	5.10	5.03	-0.07	5.25	0.15
		<chem>c(c(c(c1C1C)C)C)C(c1C)C</chem>	5.11	5.28	0.17	4.71	-0.40
		<chem>Oc(c(c(c1Cl)Cl)Cl)Cl)c1Cl</chem>	5.12	4.74	-0.38	4.99	-0.13
		<chem>OC(=O)c1cccc1Nc2c(C)c(C)ccc2</chem>	5.12	5.28	0.16	4.58	-0.54
		<chem>CCCCCCCCCCCC</chem>	5.13	4.77	-0.36	5.36	0.23
		<chem>c(ccc(c1)C)(c1)C(C)(C)C</chem>	5.17	4.45	-0.72	4.44	-0.73
		<chem>c(c(c(c1Cl)Cl)Cl)Cl)(c1)Cl</chem>	5.17	5.22	0.05	5.22	0.05
		<chem>C(CCCCC)C</chem>	5.18	4.27	-0.91	4.73	-0.45
		<chem>Oc(c(cc1C(C)(C)C(C)(C)C)c1</chem>	5.19	5.33	0.14	4.91	-0.28
		<chem>O=C(c(c(C(=O)c1c(N)c(Oc(cccc2)c2)c(Oc(cccc3)c3)c4N)ccc5)c5)c14</chem>	5.19	5.59	0.40	4.93	-0.26
		<chem>c12N(CCCN(C)C)c3ccc(Cl)ccc3CCc1cccc2</chem>	5.19	5.65	0.46	5.04	-0.15
		<chem>CC(c1c(cccc1)c2cccc2)C</chem>	5.20	5.21	0.01	5.25	0.05
		<chem>c(cccc1)(c1)C(c(cccc2)c2)(c(cccc3)c3)Cl</chem>	5.25	5.58	0.33	5.63	0.38
		<chem>CCCN(CCC)c1c(cc(cc1N(=O)(=O)C(F)(F)F)N(=O)(=O)(=O)C(F)(F)F)N(=O)(=O)</chem>	5.34	5.31	-0.03	5.09	-0.25
		<chem>N(=O)(=O)c1cc(N(=O)(=O)cc(Br)c1N=Nc2cc(OC)c(N(CC=C)CCC(#N)cc2NC(=O)C</chem>	5.40	5.34	-0.06	5.32	-0.08
		<chem>CN(C)CCCN2c1cccc1Sc3ccc(Cl)cc23</chem>	5.41	5.20	-0.21	5.18	-0.23
		<chem>O=C(OC)CCCCCCCCCCCC</chem>	5.41	5.28	-0.13	5.51	0.10
		<chem>O=C(OCCN(c(ccc(N=Nc1c(C(#N)cc(N(=O)c1)c1C(#N))c2C)c2)CCCC)C</chem>	5.50	5.83	0.33	5.38	-0.12
		<chem>O(OC(c(cccc1)c1)(C)C)C(c(cccc2)c2)(C)C</chem>	5.50	5.88	0.38	5.43	-0.07
		<chem>C(CCC(C1)C(C)C)(C1)C</chem>	5.56	4.92	-0.64	4.95	-0.61
		<chem>Oc1cc(ccc1)CCCCCCCC</chem>	5.61	5.99	0.38	6.07	0.46
		<chem>O=C(OCCCC)c(c(ccc1)C(=O)OCC</chem>	5.62	5.59	-0.03	5.55	-0.07
		<chem>CCC)c1</chem>					
		<chem>OCC=C(C=CC=C(C=CC(=C(CCC1)C)C1(C)C)C)C</chem>	5.68	7.62	1.94	6.38	0.70
		<chem>c(P(c(cccc1)c1)c(cccc2)c2)(cccc3)c3</chem>	5.69	5.02	-0.67	5.46	-0.23
		<chem>C(=C)CCCCCCCC</chem>	5.70	5.12	-0.58	5.63	-0.07
		<chem>O=C(OC)CCCCCCCCCCCC</chem>	5.71	5.78	0.07	5.95	0.24
		<chem>c(c(c(c1Cl)Cl)Cl)Cl)(c1Cl)Cl</chem>	5.73	5.86	0.13	5.70	-0.03
		<chem>O=P(Oc1cccc1)(Oc2cccc2)OCC(CC)CCCC</chem>	5.73	6.30	0.57	5.30	-0.43
		<chem>Oc(ccc(c1)CCCCCCCC)c1</chem>	5.76	5.99	0.23	6.09	0.33
		<chem>c(c(c(c1)ccc2)c2)c(c(c3ccc4)c4)C(c3C)c1</chem>	5.80	6.62	0.82	6.61	0.81
		<chem>c1ccc2ccc3c4cccc4ccc3c2c1</chem>	5.81	5.52	-0.29	5.71	-0.10
		<chem>CC(C)=CC2C(C(=O)OC1CC(=O)C(=C1C)CC=CC=C)C2(C)C</chem>	5.90	6.28	0.38	5.10	-0.80
		<chem>CSc4ccc3Sc1cccc1N(CCC2CCCCN2C)c3c4</chem>	5.90	6.45	0.55	5.93	0.03
		<chem>c1ccc(cc1)c2ccc(cc2)c3cccc3</chem>	6.03	5.52	-0.51	5.70	-0.33
		<chem>CCCCCCCCCCCCCCCC</chem>	6.03	5.75	-0.28	6.21	0.18
		<chem>Oc(c(cc1)C(C)(C)C)C(C)(C)C(c1C)C1C(C)(C)C</chem>	6.06	6.39	0.33	6.28	0.22
phenol, 2,4,6-tris(1,1-dimethylethyl)-1-tetradecanol							

dodecane	C(CCCCCCCCCC)C	6.10	6.23	0.13	6.42	0.32
tetradecanoic acid	O=C(O)CCCCCCCCCCCCC	6.11	5.98	-0.13	6.10	-0.01
octanoic acid, heptyl ester	CCCCCCCC(=O)OCCCCCCC	6.11	6.27	0.16	6.09	-0.02
heptanoic acid, octyl ester	CCCCCCCCOC(=O)CCCCC	6.11	6.27	0.16	6.10	-0.01
decanoic acid, pentyl ester	CCCCCCCC(=O)OCCCCC	6.11	6.27	0.16	6.11	0.00
butanoic acid, undecyl ester	CCCCCCCCCCCCOC(=O)CCC	6.11	6.27	0.16	6.28	0.17
benzo[a]pyrene	c(c(c(cc1)ccc2)c2cc3) (c3cc(c4ccc5)c5)c14	6.13	6.11	-0.02	6.39	0.26
cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, [5-(phenylmethyl)-3-furanyl]methyl ester	CC(C)=CC3C(C(=O)OCc2coc(Cc1ccccc1)c2)C3(C)C	6.14	7.11	0.97	5.38	-0.76
chlordanes	ClC(C(Cl)C1)C(C1C2(Cl)C=3Cl)C(Cl) (C3Cl)C2(Cl)Cl	6.22	6.26	0.04	6.02	-0.20
phenol, 2,2-methylenebis[6-(1,1-dimethylethyl)-4-methyl-	Oc(c(cc1)C)Cc(c(O)c(cc2C)C(C) (C)C)c2)c1C(C)(C)C	6.25	7.97	1.72	5.89	-0.36
1,1'-biphenyl, 2,2,4,4'-tetrachloro	Clc2c(ccc2Cl)c1c(cc(cc1)Cl)Cl	6.29	6.34	0.05	6.23	-0.06
9,12,15-octadecatrienoic acid, methyl ester	O=C(OC)CCCCCCCC=CCC=CCC=CCC	6.29	7.59	1.30	6.62	0.33
2H-benzimidazol-2-one, 1-[1-[4,4-bis(4-fluorophenyl)butyl]-4-piperidiny]-1,3-dihydro-	C(c1ccc(F)cc1) (c2ccc(F)cc2)CCCN(CC3)CCC3N4C(=O)Nc5cccc45	6.30	6.23	-0.07	6.36	0.06
retinoic acid	O=C(O)C=C(C=CC=C(C=CC(=C(CC1)C)C1(C)C)C)C	6.30	7.85	1.55	5.66	-0.64
tetradecanoic acid, methyl ester	O=C(OC)CCCCCCCCCCCCC	6.41	6.27	-0.14	6.38	-0.03
benz[j]aceanthrylene, 1,2-dihydro-3-methyl-	c(c(ccc1C)cc(c2ccc3cccc4)c34) (c1CC5)c25	6.42	7.05	0.63	6.49	0.07
9,12,15-octadecatrienoic acid	O=C(O)CCCCCCCC=CCC=CCC=C	6.46	7.30	0.84	6.62	0.16
octanoic acid, octyl ester	O=C(OCCCCCCCC)CCCCCCC	6.51	6.76	0.25	6.52	0.01
dodecanoic acid, butyl ester	O=C(OCCCC)CCCCCCCCCCC	6.51	6.76	0.25	6.61	0.10
9-hexadecenoic acid	O=C(O)CCCCCCCC=CCCCCCC	6.58	6.75	0.17	6.71	0.13
1,2-benzenedicarboxylic acid, dihexyl ester	O=C(OCCCCC)c(c(ccc1)C(=O)OC CCCC)c1	6.82	6.57	-0.25	6.28	-0.54
1,2-benzenedicarboxylic acid, butyl octyl ester	O=C(OCCCCCCCC)c(c(ccc1)C(=O) OCCCC)c1	6.82	6.57	-0.25	6.47	-0.35
9,12-octadecadienoic acid, methyl ester	O=C(OC)CCCCCCCC=CCC=CCCC CC	6.82	7.80	0.98	6.95	0.13
arachidonic acid	CCCCC=CCC=CCC=CCC=CCCC C(=O)O	6.98	8.07	1.09	6.80	-0.18
9,12-octadecadienoic acid	O=C(O)CCCCCCCC=CCC=CCCCC C	7.05	7.51	0.46	7.06	0.01
octadecadienoic acid	CCCCCCCCC=CCC=CCCCC(=O) O	7.05	7.51	0.46	7.11	0.06
hexadecanoic acid	O=C(O)CCCCCCCCCCCCCCCC	7.17	6.96	-0.21	7.23	0.06
tetradecane	C(CCCCCCCCCCCC)C	7.20	7.22	0.02	7.70	0.50
hexadecanoic acid, methyl ester	O=C(OC)CCCCCCCCCCCCCCCC	7.38	7.25	-0.13	7.41	0.03
9-octadecenoic acid, methyl ester	O=C(OC)CCCCCCCC=CCCCCCCC C	7.45	8.02	0.57	7.94	0.49
phenol, 2,2'-methylenebis[3,4,6-trichloro-]	Oc(c(c(c(c1)Cl)Cl)Cc(c(cc2Cl)Cl)Cl) c2O)c1Cl	7.54	6.92	-0.62	6.77	-0.77
1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester	O=C(OC(CCCC)CC)c(c(ccc1)C(=O))OCC(CCCC)CC)c1	7.60	8.39	0.79	7.07	-0.53
9-octadecenoic acid	O=C(O)CCCCCCCC=CCCCCCCCC	7.64	7.73	0.09	7.68	0.04
11-octadecenoic acid	O=C(O)CCCCCCCC=CCCCCCCCC	7.64	7.73	0.09	7.69	0.05
phenol, 4-dodecyl-	Oc(ccc1)CCCCCCCCCCCC)c1	7.91	7.46	-0.45	7.81	-0.10
1,2-benzenedicarboxylic acid, dioctyl ester	O=C(OCCCCCCCC)c(c(ccc1)C(=O) OCCCCCCCC)c1	8.10	8.54	0.44	7.76	-0.34
1,2-benzenedicarboxylic acid, decyl hexyl ester	O=C(OCCCCCCCCCCCC)c(c(ccc1)C(=O) O)OCCCCCCCC)c1	8.10	8.54	0.44	7.91	-0.19
octadecanoic acid	O=C(O)CCCCCCCCCCCCCCCCC	8.23	7.94	-0.29	8.02	-0.21
octadecanoic acid, methyl ester	O=C(OC)CCCCCCCCCCCCCCCCC	8.35	8.23	-0.12	8.45	0.10
benzene, dodecyl-	c(ccc1)(c1)CCCCCCCCCCCC	8.65	7.94	-0.71	8.38	-0.27
eicosanoic acid	O=C(O)CCCCCCCCCCCCCCCCC C	9.29	8.93	-0.36	8.53	-0.76