

**Outliers of logP<sub>ow</sub>**

<b>Name</b>	<b>logP<sub>ow</sub> exp</b>	<b>logP<sub>ow</sub> calc</b>	<b>Diff.</b>
Pyridine-N-oxide	-1.69	3.67	-5.36
Roxithromycin	3.79	-0.06	3.85
2-Methyl-4-nitroquinoline-1-oxide	1.25	-2.49	3.74
Azithromycin	4.02	0.29	3.73
Phthalide	0.80	3.97	-3.17
8-Azaadenine	-0.96	2.09	-3.05
Erythromycin	2.54	-0.29	2.83
2-Methylbenzaloxime	2.53	-0.21	2.74
Amitrole	-0.87	1.83	-2.70
Clarithromycin	3.16	0.70	2.46
8-Azaguanine	-0.71	1.61	-2.32
Benzaloxime	1.75	-0.54	2.29
Altretamine	2.73	0.51	2.22
Dithianon	2.84	0.62	2.22
Anilazine	3.00	5.20	-2.20
Flupyrsulfuron-methyl	1.30	3.50	-2.20
Diacetylmorphine	1.59	3.76	-2.17
2-Carboxypyridine	-1.98	0.15	-2.13
Cefatrizine	-2.24	-0.15	-2.09
Sulfamethizole	0.54	2.60	-2.06
Benzo-1,2,3-triazole	1.34	3.40	-2.06
5-Ethyl-6-azauracil	0.22	2.24	-2.02
6-Azauridine	-2.14	-4.15	2.01
p-Nonylphenyl diphenyl phosphate	5.90	7.90	-2.00
Cephalexin	0.65	-1.34	1.99
Bendiocarb	1.70	3.69	-1.99
4-Pyrimidinol	-1.38	0.60	-1.98
Carbomycin	3.04	1.06	1.98
4-Amino-3-(methylthio)-1,2,4-triazin-5-one	0.38	-1.59	1.97
Tylosin	1.63	-0.34	1.97
Oryzalin	3.73	1.83	1.90
Propiolactone	-1.36	0.53	-1.89
Spironolactone	2.78	4.66	-1.88
6-Acetylmorphine	1.55	3.40	-1.85
beta-Butyrolactone	-0.84	1.00	-1.84
Hydromorphone	0.90	2.71	-1.81
Pyrazin-2-one	-1.49	-3.29	1.80
Tazemetostat	2.82	4.60	-1.78
Cephalothin	-0.20	1.57	-1.77
Molibresib	2.80	4.55	-1.75
Etorphine	2.79	4.54	-1.75
Verapamil	3.79	5.54	-1.75
1-Hexadecyl-3-methylimidazolium bromide	10.42	8.72	1.70
Doxorubicin	0.65	-1.03	1.68
2-Aminobenzenethiol	3.00	1.32	1.68
1-Ethyl-3-methylimidazolium trifluoroacetate	1.95	0.29	1.66
Cetylpyridinium chloride	9.61	7.95	1.66
Acetaldoxime	-0.18	-1.83	1.65
Rubeanic acid	-0.44	-2.08	1.64
Profluralin	6.34	4.71	1.63
1-Pentadecanol	7.11	5.52	1.59
Pentazocine	3.31	4.90	-1.59
1-Bromodecane	6.43	4.84	1.59

Dihydro-5-methyl-2(3H)-furanone	-0.28	1.30	-1.58
6-Aminonicotinamide	0.70	-0.86	1.56
Codeine	1.19	2.75	-1.56
Colchicine	1.30	2.85	-1.55
Aldicarb	1.13	-0.42	1.55
Uric acid	-1.11	0.44	-1.55
Morphine	0.89	2.43	-1.54
Sulfadimethoxine	1.63	3.13	-1.50
5-Ethylidihydro-2(3H)-furanone	0.24	1.73	-1.49
2-Amino-4-chlorothiophenol	3.33	1.85	1.48
Valerolactone	-0.35	1.13	-1.48
Butyrolactone	-0.64	0.83	-1.47
Disopyramide	2.37	3.84	-1.47
4-Amino-1,2,4-triazole	-1.38	0.08	-1.46
7H-Benzimidazo(2,1-a)benzo(de)isoquinolin-7-one	1.76	3.22	-1.46
1-Tetradecanol	6.54	5.09	1.45
Enoxacin	2.30	0.86	1.44
O,O'-Dimethyl-O''-(benzothien-3-yl)glyoxylonitrile oximino phosphate	0.76	-0.67	1.43
Propiconazole	3.50	4.93	-1.43
Omeprazole	2.23	0.82	1.41
Tetracaine	3.73	2.34	1.39
Dihydro-3-methyl-2(3H)-furanone	-0.28	1.11	-1.39
Terazosin	2.29	0.90	1.39
Phenprocoumon	3.62	5.00	-1.38
Helenalin	0.87	2.24	-1.37
Steroid09	3.13	4.49	-1.36
1,4-Dicyanobutane	-0.32	1.04	-1.36
1-Hexadecyl-3-methylimidazolium chloride	10.08	8.72	1.36
Mirex	5.28	6.62	-1.34
Cefadroxil	-0.40	-1.74	1.34
Telmisartan	7.73	6.40	1.33
Furosemide	2.56	1.23	1.33
9-Carboxy-9,10-dihydroanthracene	2.67	4.00	-1.33
Glutaronitrile	-0.72	0.61	-1.33
1-Tridecanol	5.97	4.66	1.31
Pentafluorophenol	3.23	1.92	1.31
3-Hydroxypicolinamide	0.65	-0.65	1.30
Xamoterol	0.61	-0.69	1.30
Vinylchloride	2.79	1.50	1.29
4-Hydroxyquinoline	0.58	1.87	-1.29
5-Butyldihydro-2(3H)-furanone	1.30	2.59	-1.29
Dodecylbromide	6.98	5.70	1.28
Buprenorphine	4.82	6.10	-1.28
Ouabain	-1.70	-0.43	-1.27
Adipic dihydrazide	-2.88	-1.62	-1.26
3,4-Dimethoxythiophenol	3.32	2.06	1.26
Acarin	4.28	5.53	-1.25
4-Nitromethylhippuric acid	0.98	-0.27	1.25
Buquinolate	2.18	3.42	-1.24
Sulfapyridine	-0.02	1.21	-1.23
Dibenzoyl	3.38	2.15	1.23
Adenosine	-1.05	-2.28	1.23
Fluazuron	5.10	6.32	-1.22
1-Decanol	4.57	3.37	1.20
4-Isothiocyanatodiphenylsulfoxide	4.40	3.20	1.20

n-Octadecanoic acid	8.23	7.04	1.19
Imazalil	3.82	2.63	1.19
Mefruside	1.54	0.36	1.18
Methohexital	2.80	1.64	1.16
Chlorfenvinphos	3.10	4.26	-1.16
Primidone	0.91	2.06	-1.15
Probenecid	3.21	2.07	1.14
O,O'-Diisopropyl-O''-(2-methoxycarbonylbenzofuran-3-yl)glyoxylonitrile oximino phosphate	1.36	0.23	1.13
Cefotaxime	-1.36	-0.26	-1.10
Didanosine	-1.24	-0.16	-1.08
Doxycycline	0.42	-0.62	1.04
2,5-Dibromo-3,4-hexanedione	0.20	1.24	-1.04
Tilmicosin	3.80	2.85	0.95
Phosphoric acid	-0.77	not evaluable	
Sorbose-6-phosphate	0.38	not evaluable	
Tetrabutyl silicate	5.61	not evaluable	
Cytidine monophosphate	0.44	not evaluable	