

**Outliers of logKaw**

<b>Name</b>	<b>logKaw exp</b>	<b>logKaw calc</b>	<b>Diff</b>
Metosulam	-15.50	-6.41	-9.09
Flurtamone	-11.59	-4.94	-6.65
Tris-BP	-2.97	-8.64	5.67
Flumetsulam	-14.56	-9.13	-5.43
Pyrifthalid	-8.80	-4.60	-4.20
Phenazopyridine	-11.37	-7.22	-4.15
Fluazifop	-10.93	-6.89	-4.04
Gibberellic acid	-10.53	-14.55	4.02
profluralin	-1.92	-5.89	3.97
Nitralin	-6.18	-9.95	3.77
Thiazafurion	-7.63	-3.96	-3.67
3-Amino-1H-1,2,4-triazole	-9.60	-5.98	-3.62
fluazinam	-2.91	-6.52	3.61
flumetralin	-2.75	-6.28	3.53
Acetoacetanilide	-8.94	-5.45	-3.49
benefin	-2.04	-5.22	3.18
Triapenthenol	-8.00	-4.91	-3.09
Methomyl	-9.07	-5.99	-3.08
AKD2023	-4.45	-7.49	3.04
Isoxaflutole	-7.70	-10.74	3.04
Ferimzone	-8.25	-5.23	-3.02
fluchloralin	-2.94	-5.95	3.01
Butanedinitrile	-6.58	-3.57	-3.01
2,4-Pentanediol	-6.97	-3.99	-2.98
trifluralin	-2.25	-5.22	2.97
Quinizarin	-5.49	-8.44	2.95
ethalfuralin	-2.28	-5.22	2.94
Metaldehyde	-2.68	-5.58	2.90
isopropalin	-2.83	-5.72	2.89
Cymoxanil	-7.47	-10.33	2.86
Quizalofop-P-ethyl	-7.08	-9.91	2.83
Isoxaben	-6.85	-4.09	-2.76
prodiamine	-3.50	-6.26	2.76
Butoxycarboxim	-9.67	-12.41	2.74
Diisodecylphthalate	-2.14	-4.87	2.73
1,4-Dicyanobutane	-6.30	-3.60	-2.70
Chlorpromazine	-8.21	-5.52	-2.69
Glyoxal	-6.87	-4.18	-2.69
fenclozim	-3.14	-5.81	2.67
2-hydroxypropyl laurate	-2.37	-5.03	2.66
Musk xylene	-2.90	-5.55	2.65
Acariflor	-6.05	-8.70	2.65
Bensulfuron-methyl	-12.04	-14.65	2.61
Bromuconazole	-8.20	-5.63	-2.57
Azoxystrobin	-11.01	-8.51	-2.50
lprodione	-8.00	-10.50	2.50
Halauxifene	-8.94	-11.44	2.50
TCEP	-3.87	-6.36	2.49
4-CPA	-8.41	-5.93	-2.48
phosmet	-5.87	-8.34	2.47
Benzylaminopurine	-11.15	-8.69	-2.46
Ethychlozate	-7.60	-5.15	-2.45
Fenoxanil	-10.09	-7.65	-2.44

Desmetryn	-7.38	-9.81	2.43
Dichlorophen	-10.33	-7.92	-2.41
Diclofop	-9.36	-6.95	-2.41
Picric acid	-8.87	-6.46	-2.41
Diphacinone	-8.20	-10.59	2.39
Bis(2-ethylhexyl)terephthalate	-2.67	-5.04	2.37
Ethirimol	-6.86	-9.20	2.34
Tolprocarb	-8.21	-10.53	2.32
Diclobutrazol	-7.38	-5.10	-2.28
decachlorodiphenylether	-0.75	-3.01	2.26
Benazolin	-10.02	-7.77	-2.25
Dithianon	-9.07	-11.30	2.23
tebupirimfos	-3.73	-5.96	2.23
Tralopyril	-7.05	-4.83	-2.22
Benzo-1,2,3-triazole	-4.72	-2.51	-2.21
N-nitroso-N-methylurethane	-3.30	-1.09	-2.21
4-Nitrophenol	-7.58	-5.38	-2.20
fenpyroximate	-4.26	-6.46	2.20
Metazachlor	-7.25	-5.07	-2.18
Malonic acid	-10.16	-7.99	-2.17
Hydroquinone	-8.72	-6.57	-2.15
Phenacetin	-8.13	-6.00	-2.13
emylcamate	-2.86	-4.99	2.13
propylene carbonate	-5.54	-3.41	-2.13
cymiazole	-5.57	-3.45	-2.12
Propylenecarbonate	-5.54	-3.42	-2.12
1,1,1-trifluoroacetone	-3.50	-1.39	-2.11
Tribenuron-methyl	-9.89	-11.99	2.10
Diphenamid	-8.81	-6.71	-2.10
fluoroacetic acid	-6.30	-4.21	-2.09
Acetylsalicylic acid	-7.28	-5.20	-2.08
Haloxypop-etotyl	-7.97	-5.90	-2.07
8-Hydroxyquinoline	-4.70	-6.75	2.05
Coumatetralyl	-10.19	-8.14	-2.05
Tetrachlorocatechol	-4.85	-6.87	2.02
Fenpropathrin	-3.50	-5.51	2.01