

**Outliers of logKoa**

<b>Name</b>	<b>logKoa exp</b>	<b>logKoa calc</b>	<b>Diff</b>
Metosulam	16.74	9.29	7.45
2,2'-Azobisisobutyronitrile	4.69	12.02	-7.33
Flurtamone	14.44	8.32	6.12
Gibberellic acid	10.32	16.22	-5.90
Aldoxycarb S,S-dioxide	6.01	11.69	-5.68
Fluazinam	6.94	12.15	-5.21
Tricyclazole	10.28	5.80	4.48
Thiazopyr	8.62	13.03	-4.41
Galactitol	13.99	9.93	4.06
tau-Fluvalinate	11.43	15.43	-4.00
Decachlorodiphenyl ether	8.24	12.17	-3.93
Thiencarbazone-methyl	9.66	13.57	-3.91
Metaldehyde	2.75	6.54	-3.79
4-Cyanophenol	10.51	6.87	3.64
Flumetralin	8.37	11.76	-3.39
Bixafen	10.54	13.88	-3.34
Dodecamethylpentasiloxane	2.29	5.52	-3.23
Phenazopyridine	14.05	10.86	3.19
Quizalofop-P-ethyl	11.23	14.40	-3.17
Salicylaldehyde	8.70	5.61	3.09
Warfarin	10.34	13.37	-3.03
Phosmet	8.48	11.41	-2.93
Milbemycin a-4	16.13	19.04	-2.91
Profluralin	7.72	10.61	-2.89
Ethirimol	8.83	11.68	-2.85
Chlorpromazine	13.32	10.49	2.83
Diphacinone	12.29	15.11	-2.82
Prodiamine	7.59	10.33	-2.74
Dimethipin	8.43	5.70	2.73
Fluopicolide	10.12	12.80	-2.68
Buprofezin	8.88	11.49	-2.61
Acrinathrin	10.61	13.19	-2.58
Fluazifop	13.76	11.22	2.54
Fluchloralin	7.63	10.16	-2.53
Imazamox	14.38	16.89	-2.51
Aminocyclopyrachlor	8.91	11.38	-2.47
Metazachlor	9.14	6.67	2.47
Spiromesifen	9.46	11.91	-2.45
Daimuron	10.00	12.43	-2.43
Chloridazon	12.85	10.44	2.41
Thiazafluron	9.22	6.82	2.40
Paraldehyde	3.09	5.44	-2.35
Benfluralin	7.50	9.81	-2.31
Oxadixyl	10.12	7.81	2.31
Chlorflurenol-methyl	9.17	11.42	-2.25
Fenoxanil	13.32	11.07	2.25
Valifenalate	11.63	13.86	-2.23
Diclofop	13.75	11.57	2.18
4-CPA	10.11	7.94	2.17
Isoxaflutole	9.77	11.93	-2.16
4-Nitrophenol	9.23	7.09	2.14
Imazaquin	15.88	18.01	-2.13
Fluoxastrobin	12.91	10.79	2.12

Hydroprene	9.36	7.24	2.12
8-Hydroxyquinoline	6.57	8.67	-2.10
Dicyclopentadiene	3.18	5.27	-2.09
Isoxaben	10.64	8.56	2.08
Nuarimol	9.94	12.00	-2.06
Perfluoroethane	-0.69	1.37	-2.06
Bendiocarb	7.14	9.19	-2.05
Flumetsulam	13.19	11.14	2.05
Ethalfuralin	7.53	9.55	-2.02
Quizalofop-Ethyl	10.72	12.74	-2.02
Methomyl	8.80	6.79	2.01
Lactofen	10.58	12.56	-1.98
Fuberidazole	11.07	9.10	1.97
Dichlorprop	10.68	8.72	1.96
Dimethirimol	8.81	10.76	-1.95
Fampridine	7.99	6.06	1.93
MCPA	10.28	8.36	1.92
Fluoroimide	5.49	7.38	-1.89
Trifluralin	7.93	9.81	-1.88
Dichlorophen	14.33	12.48	1.85
Triflumizole	10.90	9.06	1.84
Propetamphos	9.14	7.32	1.82
1-Methylindole	6.76	4.96	1.80
6-Hydroxy-2,2',3,3',4,6'-hexabromodiphenylether	12.30	14.10	-1.80
Bensulfuron-methyl	14.38	16.17	-1.79
1,2-Phenylenediamine	5.64	7.43	-1.79
Phenacetin	9.59	7.82	1.77
2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether	9.81	11.56	-1.75
Ethametsulfuron-methyl	14.28	16.02	-1.74
Furametpyr	12.18	13.92	-1.74
Propanil	10.38	8.64	1.74
2,2',3,4,4',5',6-Heptabromodiphenylether	14.40	12.67	1.73
Diallate	8.84	7.11	1.73
Pefurazate	9.46	11.19	-1.73
3-Nitrophenol	8.81	7.09	1.72
Iprovalicarb	11.69	13.40	-1.71
Iprodione	10.76	12.46	-1.70
5-Hydroxy-2,2',4,4',5'-pentabromodiphenylether	11.47	13.17	-1.70
Benodanil	9.57	11.26	-1.69
Tembotrione	12.47	14.16	-1.69
Tribenuron-methyl	11.09	12.77	-1.68
Salithion	4.98	6.66	-1.68
3-Cyanophenol	8.43	6.80	1.63
4-Nitroaniline	8.41	6.79	1.62
Benzylaminopurine	12.86	11.24	1.62
2,4-D	10.15	8.54	1.61
Bis(2-ethylhexyl)phthalate	10.48	12.09	-1.61
Diclobutrazol	11.00	9.40	1.60
Picric acid	9.99	8.39	1.60
4-Hydroxybenzaldehyde	8.75	7.15	1.60
Trinexapac-ethyl	7.92	9.49	-1.57
2'-Hydroxy-2,3',4,5'-tetrabromodiphenylether	10.68	12.24	-1.56
Triazamate	10.75	12.30	-1.55
Butanedinitrile	5.16	3.61	1.55
Maleic hydrazide	9.01	7.46	1.55

2,2-Dichloroethanol	3.14	4.68	-1.54
Chlordecone	10.87	9.33	1.54
2,4-Dinitrophenol	6.98	8.51	-1.53
4-Hydroxy-3-nitrobenzaldehyde	5.53	7.03	-1.50
2,2',3,3',4,4',5,5'-Octachlorodiphenyl ether	9.47	10.96	-1.49
Imazalil	10.38	8.89	1.49
Ethyl 4-(4-chloro-2-methylphenoxy)butanoate	9.15	7.67	1.48
Trichloroacetonitrile	2.34	3.81	-1.47
2,2,2-Trifluoroethylacetate	1.56	3.02	-1.46
Azinphos-methyl	10.83	9.38	1.45
trans-Azobenzene	7.06	8.49	-1.43
Cymoxanil	7.75	9.18	-1.43
3,5-Dichlorophenol	8.28	6.86	1.42
Cyhalofop-butyl	9.23	10.64	-1.41
5-Hydroxy-2,2',4,4'-tetrabromodiphenylether	10.82	12.23	-1.41
N-Methyl-N-nitrosobenzenemethanamine	5.15	6.56	-1.41
6-Hydroxy-2,2',4,4'-tetrabromodiphenylether	10.83	12.23	-1.40
Fenpropathrin	9.37	10.77	-1.40
Dichloroacetic acid	7.14	5.76	1.38
p-tert-Butylphenyl diphenyl phosphate	9.62	10.94	-1.32
Amitraz	10.11	9.04	1.07
Imidacloprid	12.94	not calc.	
Nitroguanidine	11.93	not calc.	