number	CAS	NAME	MLOGP	TerraQSAR-LOGP	CLOGP (Daylight)	KOWWIN (1.67)	SciLogP
1	4368-28-9	tetrodotoxin; tetrodin	-	-1.01	-3.87	-7.10	-2.24
2	38304-91-5	minoxidil	1.24 *	1.38	-0.72 (see note a)	1.35	0.96
3	2051-24-3	decachlorobiphenyl	8.27	8.18	9.92	10.20	5.04
4	2386-56-3	potassium methylsulfonate	-	-1.91	-6.12	-4.53	-0.84
5	140-01-2	DTPA pentasodium	-	-3.05	-14.05	-16.25	1.37
6	143-50-0	kepone hydrate	-	4.86	1.73	5.22	3.19
7	13176-69-7	siloxane; MD3OH	-	5.15	0.64	3.98	3.42
8	53994-73-3	cefaclor	-1.79 *	-1.79	-1.64	0.70	2.43
9	1085-12-7	heptyl 4-hydroxybenzoate	4.83 *	4.83	5.16	4.94	4.60
10	4474-91-3	angiotensin II	-	2.16	-4.93	-1.16	-1.31
11	19772-79-3	vobtusine	-	2.20	2.34	unable	4.12
12	67-56-1	methanol	-0.77 *	-0.74	-0.77	-0.63	-0.66
13	558-13-4	carbon tetrabromide	3.42 *	3.42	3.44	2.80	3.44
14	87-68-3	hexachloro-1,3-butadiene	4.78 *	4.78	4.90	4.71	5.29
15	67696-82-6	acrihellin	-	2.54	2.80	3.31	3.66
16	162795-98-4	DTX4; shellfish poison	-	2.06	2.25	2.36	-1.39
17	11050-21-8	ciguatoxin P-CTX-1 (Pacific variety)	-	2.24	-2.54	unable	3.63
18	68-26-8	vitamin A	5.68 *	5.68	6.40	7.62	5.72
19	19772-79-3	vobtusin	-	2.20	2.34	unable	4.12
20	75-76-3	tetramethylsilane	3.24 *	3.23	3.24	2.72	2.07
21	41198-08-7	profenofos	4.68 *	4.68	4.67	4.82	4.04
22	5234-68-4	vitavax; carboxin	2.14 *	2.14	2.14	1.49	2.11
23	13909-09-6	semustine; 1-(2-chloroethyl)-3-(4-methylcyclohexyl)-1-nitrosourea; methyl-CCNU	3.30 *	3.30	3.27	3.38	2.18
24	76129-15-2	NSC-309697; colchicine, 10-(benzylamino)-10-demethoxy-	3.58 *	1.32	2.51	3.81	2.79
25	41575-94-4	Carboplatin; CBDCA	-2.53 to -0.16	-1.33	-0.34	structure wrong (-0.46)	3.55

Note a: Daylight claims a CLOGP (v. 4.71) value of 0.541 (all fragments measured), however the program at their website results in a value of -0.72.

number	SMILES
1	[C@@]23([H])[C@@]([C@]4([H])[C@]1([H])C(O)N=C(N)N[C@@]1(C2O)C(O)[C@](O3)(O)O4)(CO)O
2	C1CCCCN1C2=NC(N)=[N+]([O-])C(N)=C2
3	Clc1c(Cl)c(Cl)c(c(Cl)c1Cl)c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl
4	[K+].[O-]S(=O)(=O)C
5	[Na+].[O-]C(CN(CCN(CCN(CC([O-])=O)CC([O-])=O)CC([O-])=O)CC([O-])=O)=O.[Na+].[Na+].[Na+].[Na+]
6	[C@]15(Cl)C(Cl)(Cl)[C@@]3([C@@]2(Cl)[C@]1([C@@]4(Cl)C(O)(O)[C@@]2([C@]3(Cl)[C@]45Cl)Cl)Cl)Cl
7	O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C
8	O=C2N1/C(=C(/Cl)CS[C@]1([H])[C@@]2([H])NC(=O)[C@@](N)([H])C=3C=CC=CC=3)C(O)=O
9	O=C(OCCCCCCC)c(ccc(O)c1)c1
10	O/C1=C/C=C(C=C1)C[C@]([H])(NC(=O)[C@@]([H])(NC(=O)[C@@]([H])(NC(=O)[C@]([H])(N)CC(O)=O)CCCNC(N)=N)C(C)(C)[H])C(=O)N[C@@]([H])(C(=O)N[C@@]([H])(C/C2=C/N=CN2)C(=O)N3CCC[C@@]3([H])C(=O)N[C@@]([H])(C/C4=C/C=CC=C4)C(O)=O)[C@](C)([H])CC
11	c1cccc2[C@]34CCN5C[C@]6([C@]7([H])OCC[C@@]7([C@@]35[H])CC(C(=O)OC)=C4Nc12)CN9c%10c(OC)cccc%10[C@@]8%11CCN%12CC[C@]%13([H])OCCC%13([C@]%11%12[H])C[C@@]([H])(C6)[C@@]89O
12	CO
13	C(Br)(Br)(Br)Br
14	C(=C(C(=C(Cl)Cl)Cl)Cl)(Cl)Cl
15	O[C@]45CC[C@]1([H])[C@]([H])(CC[C@@]2(C)[C@@]1(O)CC[C@]2([H])C=3C=CC(=O)OC=3)[C@]4(CC[C@]([H])(C5)OC(=O)C=C(C)C)C=O
16	OS(=O)(=O)SOCC(O)C(OS(=O)(=O)O)C(O)CC(OS(=O)(=O)O)CC(O)CCC([H])=C([H])CC(=O)OCCC([H])=CC=C(C)COC(=O)C(C)(O)CC1CCC(O)C2(O1)C=C(C)CC(O2)C(C)C=CC1CCC2(O1)CCC3OC(C(=C)C(O)C3O2)C(O)CC(C)C1C(C)CCC2(O1)OCCCC2
17	OC[C@](O)([H])C=CC1C=CCC2OC3CC4OC5C=CC6OC7CC(O)C8(C)OC9CC(C)CC%10OC%11C(C)C(O)C%12OC%13(OCC(O)C%13)C(C)C(C)C%12OC%11CC%10OC9CC8OC7CC=CCC6OC5C=CC4OC3C(O)C2O1
18	OC/C=C(/C=C/C=C(/C=C/C(=C(CCC1)C)C1(C)C)C)C
19	c1cccc2[C@]34CCN5C[C@]6([C@]7([H])OCC[C@@]7([C@@]35[H])CC(C(=O)OC)=C4Nc12)CN9c%10c(OC)cccc%10[C@@]8%11CCN%12CC[C@]%13([H])OCCC%13([C@]%11%12[H])C[C@@]([H])(C6)[C@@]89O
20	C[Si](C)(C)C
21	CCCSP(=O)(OCC)Oc1ccc(Br)cc1Cl
22	CC1=C(SCCO1)C(=O)Nc2ccccc2
23	C[C@]1([H])CC[C@]([H])(CC1)NC(=O)N(CCCl)N=O
24	COC=4C=3C2=C/C=C(/NC/C1=C/C=CC=C1)C(=O)C=C2[C@]([H])(CCC=3/C=C(/OC)C=4OC)NC(=O)C
25	[Pt]1([O-]C(=O)C3(CCC3)C(=O)[O-]1)([N+])[N+]