

Table 2: Dataset of Molecular Descriptors and Permeability Coefficients

Compound	Molecular Weight	Log Kow	Balaban Index	Harary Index	ForgottenIndex	logkp
aldosterone	360.44	1.08	1.74	5.65	41.0	-5.52
amobarbital	226.27	1.96	2.87	3.67	25.0	-2.64
atropine	289.38	1.81	1.63	4.69	33.5	-5.07
barbital	184.19	0.65	3.01	3.08	22.0	-3.95
benzyl alcohol	108.13	1.1	2.83	2.0	15.5	-2.22
4-bromophenol	173.01	2.59	3.03	1.83	15.5	-1.44
butanoic acid (butyric acid)	88.1	0.79	2.83	1.58	4.0	-3.0
n-butanol	74.12	0.88	2.19	1.5	7.0	-2.6
2-butanone	72.1	0.28	2.85	1.33	24.0	-2.35
butobarbital	212.24	1.65	2.89	3.58	16.5	-3.71
2-chlorophenol	128.56	2.15	3.13	1.86	15.5	-1.48
4-chlorophenol	128.56	2.39	3.03	1.83	15.5	-1.44
chloroxyleneol	156.61	3.39	3.31	2.22	17.5	-1.28
chlorpheniramine	274.8	2.7	2.26	4.31	35.0	-2.66
codeine	299.3	0.89	1.82	4.62	36.5	-4.31
cortexolone (11-desoxy-17-hydroxycorticosterone)	346.45	2.52	2.3	4.67	42.0	-4.13
cortexone (deoxycorticosterone)	330.45	2.88	2.24	4.44	41.0	-3.35
corticosterone	346.45	1.94	1.7	5.28	37.0	-4.22
cortisone	360.46	1.42	1.75	5.44	41.0	-5.0
o-cresol	108.14	1.95	3.13	1.86	15.5	-1.8
m-cresol	108.14	1.82	3.08	1.83	15.5	-1.82
p-cresol	108.14	1.95	3.03	1.83	15.5	-1.75
n-decanol	158.28	4.0	2.69	3.0	10.0	-1.1
2,4-dichlorophenol	127.55	3.08	3.17	2.03	16.5	-1.22
diethylcarbamazine	199.29	1.89	2.44	3.39	17.0	-3.89
digitoxin	764.92	1.86	0.83	11.16	67.0	-4.89
ephedrine	165.23	1.03	2.71	2.89	19.5	-2.23
?-estradiol	272.37	2.69	1.71	4.15	30.5	-3.52
estriol	288.37	2.47	1.71	4.35	31.5	-4.4
estrone	270.36	2.76	1.73	4.15	33.5	-2.44
ethanol	46.07	-0.31	1.63	1.0	2.0	-3.1
ethyl benzene	106.12	3.15	2.83	2.0	9.0	3.15
ethyl ether	74.12	0.83	2.19	1.5	15.5	1.8
4-ethylphenol	122.17	2.4	2.88	2.17	4.0	-1.46
etorphine	411.5	2.76	1.66	6.26	16.5	-2.1
fentanyl	336.5	4.37	1.57	5.75	45.5	-3.15
fluocinonide	494.55	3.19	1.62	7.06	45.0	-2.77
heptanoic acid (enanthic acid)	130.18	2.5	2.83	2.33	54.0	-1.7
n-heptanol	116.2	2.72	2.53	2.25	11.0	-1.5
hexanoic acid (caproic acid)	116.16	1.9	2.82	2.08	7.0	-1.85
n-hexanol	102.18	2.08	2.45	2.0	10.0	-1.89
hydrocortisone	362.47	1.53	1.74	5.44	6.0	-5.52
hydrocortisone-21-yl-N,N dimethyl succinamate	489.6	2.03	1.51	7.69	38.0	-4.17
hydrocortisone-21-yl-hemipimelate	504.6	3.26	1.41	7.75	47.0	-2.75
hydrocortisone-21-yl-hemisuccinate	462.5	2.11	1.53	7.0	63.0	-3.2
hydrocortisone-21-yl-hexanoate	460.6	4.48	1.52	6.75	60.0	-1.75
hydrocortisone-21-yl-octanoate	488.7	5.49	1.44	7.25	54.0	-1.21

hydrocortisone-21-yl-propionate	418.5	3.0	0.0	6.0	54.0	-2.47
hydromorphone	285.3	1.25	1.83	4.29	49.0	-4.82
hydroxyprogrenolone	330.45	3.0	2.3	4.67	35.5	-3.22
17a-hydroxyprogesterone	330.45	2.74	1.67	4.91	42.0	-3.22
isoquinoline	129.15	2.03	2.89	2.28	36.0	-1.78
meperidine	247.0	2.72	2.31	4.17	24.75	-2.43
methanol	32.04	-0.77	1.0	1.0	29.5	-3.3
methyl-[hydrocortisone-21-yl succinate	476.6	2.58	0.0	7.25	1.0	-3.68
methyl-4-hydroxy benzoate	152.14	1.96	2.75	2.86	61.0	-2.04
morphine	285.3	0.62	1.84	4.29	22.5	-5.03
2-naphthol	144.16	2.84	2.83	2.44	35.5	-1.55
naproxen	230.26	3.18	2.48	3.83	25.75	-3.4
nicotine	162.23	1.17	2.19	2.72	34.75	-1.71
nitroglycerine	227.09	2.0	3.99	3.5	20.5	-1.96
3-nitrophenol	139.11	2.0	3.07	2.28	23.0	-2.25
4-nitrophenol	139.11	1.96	3.0	2.28	20.5	-2.25
n-nitrosodiethanolamine	134.13	-1.05	3.29	2.5	20.5	-5.22
n-nonanol	144.26	3.62	2.65	2.75	11.0	-1.22
octanoic acid (caprylic acid)	144.21	3.0	2.84	2.58	9.0	-1.6
n-octanol	130.23	2.97	2.6	2.5	12.0	-1.28
ouabain	584.64	-1.51	1.28	8.53	8.0	-6.11
pentanoic acid (valeric acid)	102.13	1.3	2.82	1.83	52.0	-2.7
n-pentanol	88.15	1.56	2.34	1.75	9.0	-2.22
phenobarbital	232.23	1.47	2.54	3.88	5.0	-3.34
phenol	94.11	1.46	3.02	1.67	34.5	-2.09
pregnenolone	316.47	3.13	1.66	4.75	14.5	-2.82
progesterone	314.45	3.77	1.67	4.75	32.0	-2.82
n-propanol	60.1	0.25	1.97	1.25	35.0	-2.85
resorcinol	110.11	0.8	3.08	1.83	3.0	-3.62
salicylic acid	138.12	2.26	3.15	2.31	15.5	-2.2
scopolamine	303.35	1.24	1.42	4.78	20.5	-4.3
styrene	104.1	2.95	2.99	2.0	35.5	-0.19
sucrose	342.3	-2.252	2.18	5.29	18.5	-5.28
sufentanyl	387.5	4.59	1.74	6.26	24.0	-1.92
testosterone	288.41	3.31	1.69	4.31	45.75	-3.4
thymol	150.21	3.34	3.09	2.47	30.0	-1.28
2,4,6-trichlorophenol	162.0	3.69	3.31	2.22	17.5	-1.23
water	18.01	-1.38	0.0	0.0	0.0	-3.3
3,4-xylenol	122.17	2.35	3.17	2.03	22.5	-1.44