

Supplemental information: molecular descriptors

New alternatives for estimating the octanol/water partition coefficient and water solubility for volatile organic compounds using GLC data (Kováts retention indices)

Felicia Spafiu,^a Alice Mischie,^a Petre Ionita,^a Adrian Beteringhe,^a Titus Constantinescu,^a
and Alexandru T. Balaban^{b,*}

^a*Institute of Physical Chemistry “Ilie Murgulescu” of the Romanian Academy, Splaiul
Independentei 202, 060021 Bucharest, Romania*

^b*Texas A&M University at Galveston, 5007 Avenue U, Galveston, TX 77551, USA*

E-mail: balabana@tamug.edu, titelconstantinescu@yahoo.com

	Compound	logP _{exp}	logS _w	I	lgMr/st	nBt	Sp	V
1	ethane	1.81	-2.70	200	0.02	7	0	0
2	propane	2.36	-2.85	300	0.05	10	0	0
3	n-butane	2.89	-2.98	400	0.09	13	0	0
4	n-pentane	3.39	-3.28	500	0.13	16	0	0
5	n-hexane	4	-3.96	600	0.17	19	0	0
6	n-heptane	4.5	-4.47	700	0.2	22	0	0
7	n-octane	5.15	-5.24	800	0.24	25	0	0
8	n-nonane	5.65	-5.77	900	0.27	28	0	0
9	n-decane	6.25	-6.44	1000	0.3	31	0	0
10	n-undecane	6.54	-7.55	1100	0.33	34	0	0
11	n-dodecane	6.8	–	1200	0.35	37	0	0
12	n-tridecane	7.5	–	1300	0.38	40	0	0
13	n-tetradecane	8	–	1400	0.4	43	0	0
14	2-methylpropane	2.76	-3.08	358	0.12	13	0	0
15	3-methylheptane	–	-5.16	774	0.25	25	0	0
16	2,4-dimethylpentane	–	-4.26	608	0.24	22	0	0
17	ethene	1.13	-2.33	270	0.05	5	0	0
18	propene	1.77	-2.32	360	0.06	8	0	0
19	1-butene	2.4	-2.40	450	0.1	11	0	0
20	1-pentene	2.8	-2.68	552	0.13	14	0	0
21	1-hexene	3.4	-3.23	614	0.17	17	0	0
22	1-heptene	3.99	-3.73	723	0.2	20	0	0
23	1-octene	4.57	-4.44	819	0.24	23	0	0

24	Z-2-octene	4.44	–	849	0.23	23	0	0
25	2-ethylhexene	4.31	–	824	0.25	23	0	0
26	2-butyne	1.46	–	587	-0.08	9	0	0
27	1-octyne	3.57	–	907	0.13	21	0	0
28	2-octyne	3.57	–	979	0.14	21	0	0
29	benzene	2.15	-1.61	833	-0.04	12	0	0
30	toluene	2.73	-2.24	938	0.03	15	0	0
31	ethylbenzene	3.15	-2.80	1035	0.09	18	0	0
32	styrene	2.95	-2.53	1094	0.09	16	0	0
33	ethynylbenzene	2.4	-2.35	1096	-0.03	14	0	0
34	<i>o</i> -xylene	3.12	-2.78	1046	0.1	18	0	0
35	<i>m</i> -xylene	3.2	-2.82	1050	0.1	18	0	0
36	<i>p</i> -xylene	3.15	-2.82	1041	0.1	18	0	0
37	mesitylene	3.42	-3.40	1155	0.15	21	0	0
38	α -pinene	4.83	-4.74	1015	0.24	27	0	0
39	cyclohexane	3.44	–	735	0.03	18	0	0
40	methanol	-0.77	1.49	522	-0.36	5	28.79	1
41	ethanol	-0.31	1.34	587	-0.24	8	23.99	1
42	1-propanol	0.25	1.22	703	-0.15	11	23.83	1
43	1-butanol	0.88	-0.07	820	-0.07	14	24.15	1
44	1-pentanol	1.56	-0.60	929	-0.01	17	23.99	1
45	1-hexanol	2.03	-1.24	1032	0.05	20	24.15	1
46	1-heptanol	2.72	-1.84	1138	0.1	23	24.15	1
47	1-octanol	3.07	-2.38	1241	0.15	26	24.15	1
48	1-nonanol	4.02	-3.01	1350	0.19	29	24.15	1
49	1-decanol	4.57	-3.63	1439	0.22	32	24.15	1
50	1-undecanol	4.72	-3.96	1569	0.26	35	24.15	1
51	1-dodecanol	5.13	-4.67	1678	0.29	38	24.15	1
52	2-methyl-1-butanol	1.16	-0.47	886	0.02	17	18.47	1
53	3-methyl-1-butanol	1.42	-0.52	885	0.02	17	23.43	1
54	allyl alcohol	0.17	1.23	715	0.06	9	24.31	1
55	<i>E</i> -2-hexen-1-ol	1.6	–	1046	0.04	18	24.31	1
56	2-butanol	0.61	0.39	737	-0.03	14	20.79	1
57	2-hexanol	1.76	-0.87	950	0.07	20	16.98	1
58	2-propanol	0.05	1.22	613	-0.11	11	21.83	1
59	3-hexanol	1.65	–	941	0.07	20	12.94	1
60	2-methyl-2-propanol	0.35	1.13	654	-0.03	14	20.31	1
61	2-methyl-2-butanol	0.89	0.05	771	0.03	17	19.83	1
62	2-methyl-2-pentanol	1.39	–	868	0.08	20	19.43	1

63	3-methyl-3-pentanol	1.53	–	900	0.08	20	14.31	1
64	3-methyl-3-heptanol	–	-1.74	1078	0.22	26	18.47	1
65	α -terpineol	2.98	-2.34	1426	0.15	29	15.03	1
66	dimethylcyclohexanol	2.37	–	1173	0.16	25	15.51	1
67	cyclopentanol	0.78	0.18	996	-0.1	16	21.91	1
68	acetaldehyde	-0.22	1.36	541	-0.18	6	41.58	1
69	propionaldehyde	0.3	0.72	656	-0.1	9	41.58	1
70	butyraldehyde	0.83	-0.01	753	-0.03	12	41.58	1
71	hexanal	1.89	-1.25	966	0.08	18	41.58	1
72	heptanal	2.42	-1.96	1066	0.12	21	41.58	1
73	octanal	2.95	-2.36	1167	0.17	24	41.58	1
74	2-methyl-1-propanal	0.83	–	706	-0.01	12	35.43	1
75	propenal	-0.01	0.58	659	-0.1	7	42.06	1
76	<i>E</i> -2-butenal	0.52	0.41	870	-0.04	10	41.9	1
77	<i>E</i> -2-hexenal	1.58	–	1077	0.07	16	41.9	1
78	benzaldehyde	1.5	-1.64	1272	-0.07	14	35.83	1
79	acetone	-0.24	1.23	652	-0.07	9	38.7	1
80	2-butanone	0.29	0.49	764	-0.01	12	37.74	1
81	2-pentanone	0.91	-0.30	857	0.05	15	37.74	1
82	2-hexanone	1.38	-0.76	966	0.1	18	38.22	1
83	2-heptanone	1.98	-1.42	1061	0.14	21	38.38	1
84	2-octanone	2.37	-2.15	1165	0.18	24	38.38	1
85	2-nonanone	3.14	-2.58	1264	0.22	27	38.38	1
86	2-decanone	3.73	-3.31	1366	0.25	30	38.38	1
87	2-undecanone	4.09	-3.94	1469	0.29	33	38.38	1
88	2-dodecanone	4.55	–	1571	0.32	36	38.38	1
89	3-hexanone	1.45	-0.83	945	0.1	18	23.27	1
90	cyclopentanone	0.38	–	1050	-0.17	14	23.67	1
91	cyclohexanone	0.81	-0.59	1160	-0.07	17	38.86	1
92	cycloundecanone	3.66	–	1757	0.24	32	34.47	1
93	cyclododecanone	4.1	–	1875	0.28	35	37.5	1
94	acetophenone	1.58	-1.29	1387	0.03	17	30.87	1
95	carvone	2.52	-2.06	1566	0.18	25	29.51	1
96	acetic acid	-0.17	1.22	734	-0.39	7	63.33	1
97	propionic acid	0.33	1.13	886	-0.27	10	56.62	1
98	butyric acid	0.79	-0.17	985	-0.17	13	56.78	1
99	valeric acid	1.39	-0.63	1108	-0.08	16	56.3	1
100	hexanoic acid	1.92	-1.05	1233	-0.02	19	56.14	1
101	heptanoic acid	2.42	-1.66	1358	0.04	22	56.78	1

102	octanoic acid	3.05	-2.26	1483	0.09	25	56.78	1
103	nonanoic acid	3.42	-2.75	1608	0.14	28	56.62	1
104	decanoic acid	4.09	-3.45	1733	0.18	31	56.46	1
105	undecanoic acid	4.42	-3.55	1858	0.22	34	56.62	1
106	dodecanoic acid	4.6	-4.62	1982	0.25	37	52.62	1
107	2-methylpropionic acid	0.94	0.28	945	-0.14	13	50.7	1
108	2-methylbutyric acid	1.18	-0.36	1094	-0.06	13	53.18	1
109	3-methylbutyric acid	1.16	-0.40	1042	-0.06	16	52.78	1
110	4-methylpentanoic acid	1.79	–	1148	0	19	56.3	1
111	methyl acetate	0.18	0.52	666	-0.09	10	55.02	1
112	ethyl acetate	0.73	-0.04	751	-0.02	13	49.26	1
113	2-methylbutyl acetate	2.29	–	1058	0.13	22	49.1	1
114	propyl acetate	1.24	-0.73	844	0.04	16	50.06	1
115	butyl acetate	1.82	-1.14	958	0.09	19	48.62	1
116	3-methylbutyl acetate	2.25	-1.81	1010	0.15	22	48.86	1
117	propyl butyrate	2.15	-1.91	1024	0.13	22	32.47	1
118	methyl propionate	0.82	-0.15	770	-0.02	13	48.62	1
119	propyl formate	0.83	-0.60	762	-0.05	13	54.22	1
120	isobutyl isobutyrate	2.48	-2.16	1012	0.21	25	27.19	1
121	isopentyl isovalerate	3.62	–	1217	0.27	31	26.47	1
122	benzyl acetate	1.96	-1.69	1378	0.07	21	42.86	1
123	methyl benzoate	2.23	-1.81	1442	0.02	18	28.63	1
124	1-florooctane	4.2	-3.76	972	0.25	25	37.18	0
125	1-bromoethane	1.61	-1.08	665	-0.08	7	85.28	0
126	1-bromopentane	3.37	-3.08	973	0.09	16	79.44	0
127	2-bromooctane	4.89	-4.49	1214	0.22	25	70.74	0
128	iodomethane	1.51	-1.01	698	-0.14	4	104.46	0
129	1-iodobutane	3.08	-2.96	989	0.05	13	92.96	0
130	2-iodobutane	3.05	-2.94	946	0.07	13	84.22	0
131	1-chlorohexane	3.66	-3.12	968	0.15	19	65.5	0
132	<i>o</i> -chlorotoluene	3.42	–	1273	0.05	15	60.47	0