The solubility of liquid and solid compounds in dry octan-1-ol

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Abstract

Using literature data on solubilities, equations have been constructed for the correlation of solubilities of liquids and solids in dry octanol, as $\log S_{oct}(\text{mol/L})$. The best equation statistically uses Abraham descriptors together with the compound melting point. For 282 compounds the equation standard deviation is no more than 0.47 log units. If the melting point term is omitted the standard deviation rises to 0.63 log units. It is suggested that if Abraham descriptors are available, these equations represent the most satisfactory equations for the correlation and estimation of solubilities in dry octanol. If these descriptors are not available, then the simple equation of Yalkowsky can be used, although for 223 compounds the equation standard deviation rises to 0.71 log units.

Keywords: Solubility; octan-1-ol; Abraham descriptors, Water-octanol partition coefficient, Hydrogen bonding.

1. Introduction

The solubility of liquid and solid compounds in octan-1-ol has attracted considerable attention, no doubt due to its importance in environmental and medicinal research. Solubility in octanol is one of the physico-chemical properties that are of importance for modeling the transport and fate of chemicals in the environment (Li et al., 2003) and has been suggested as an indicator of storage capacity in natural lipids (Anliker and Moser 1987). Not surprisingly, there have been a number of methods put forward for the correlation and prediction of octanol solubility of liquids and solids

(Li, Pinsuwan and Yalkowsky, 1995; Sepassi and Yalkowsky, 2006; Admire and Yalkowsky, 2013; Raevsky and Schaper, 2008; Raevsky, Perlovich and Schaper, 2007). It is important to note that all this work refers to dry octanol; it is well-known that solubilities in wet (water-saturated) octanol and dry octanol are not the same (Bernazzani, Cabani, Conti and Mollica, 1995; Kristl and Vesnaver, 1995; Martínez and Gómez, 2001), possibly because the microscopic structure of wet and dry octanol are not the same (Chen and Siepmann, 2006).

Two extraordinarily simple equations have been constructed (Admire and Yalkowsky, 2013) for the correlation of solubilities in octanol, as $\log S_{oct}(\text{mol/L})$ and $\log S_{oct}(\text{g/L})$:

$$\log S_{oct}(\text{mol/L}) = 0.50 - 0.01(\text{mp}-25) \quad (1)$$

$$N = 223, SD = 0.71$$

$$\log S_{oct}(\text{g/L}) = 2.70 - 0.01 (\text{mp}-25) \quad (2)$$

$$N = 223, SD = 0.67$$

In eq. (1) and eq (2), the compound melting point, mp, is in $^{\circ}\text{C}$; for liquids it is taken as 25, so that the term (mp-25) is zero. N is the number of data points, that is the number of compounds, and SD is the standard deviation (calculated in this work). Other statistics that we shall use are R the correlation coefficient, F the F-statistic, and the leave-one-out Q^2 . Rather more complicated equations, eq (3) and eq (4), were proposed (Raevsky, Perlovich and Schaper, 2007) but lead to statistics no better than the simple equation, eq (1). The descriptors used in eq. (3) and eq (4) are α the compound molecular polarizability, ΣCa the overall hydrogen bond basicity (hydrogen bond acceptor) and ΣCd the overall hydrogen bond acidity (hydrogen bond donor).

$$\log S_{oct}(\text{mol/L}) = 0.45 - 0.027 \alpha - 0.22 \Sigma Ca + 0.09 \Sigma Cd \quad (3)$$

$$N = 218, SD = 0.94, R^2 = 0.457, F = 60.0, Q^2 = 0.432$$

$$\log S_{oct}(\text{mol/L}) = 1.11 - 0.013 \alpha - 0.20 \Sigma Ca - 0.0084 (\text{mp}-25) \quad (4)$$

$$N = 217, SD = 0.70, R^2 = 0.687, F = 155.8, Q^2 = 0.663$$

Because of the poor statistics of eq (3) and eq (4) another approach altogether was developed (Raevsky, Perlovich and Schaper, 2007) using a similarity principle. In order to estimate $\log S_{oct}(\text{mol/L})$ for a given compound, the data base of compounds is surveyed and a compound (or

compounds) as similar as possible to the given compound is selected. Then the solubility of the given compound is calculated from the similar compound (*pen*) through eq (5). Unfortunately, the presented statistics for eq (5) were only those for solubilities calculated from the ‘best predictors’ that is for 158 compounds out of the 218 compounds fitted by eq. (3) and eq (4). Even so, results from eq (5) do not seem to be significantly better than those from the very simple eq (1) and so an additional melting point descriptor was added, leading to eq (6). Now the statistics are markedly better, although they still refer to the “best” 158 compounds out of 218.

$$\text{Log } S_{oct}(\text{mol/L}) = \text{Log } S_{oct}(\text{mol/L})_{pen} - 0.062 (\alpha - \alpha_{pen}) - 0.14 (\Sigma Cd - \Sigma Cd_{pen}) \quad (5)$$

$$N = 158, SD = 0.66, R^2 = 0.709, F = 380.1, Q^2 = 0.701$$

$$\text{Log } S_{oct}(\text{mol/L}) = \text{Log } S_{oct}(\text{mol/L}) \text{ calc from eq. (5)} - 0.00934 (\text{mp} - \text{mp}_{pen}) \quad (6)$$

$$N = 158, SD = 0.46, R^2 = 0.865, F = 999.0, Q^2 = 0.723$$

It has been suggested (Raevsky, Perlovich and Schaper, 2007) that the experimental error in $\log S_{oct}(\text{mol/L})$ is about 0.4; if this is correct, then an SD value of 0.46 as obtained with eq (6) might be as good as it is possible to obtain. Our aim in this work was to ascertain if moderately simple equations on the lines of eq.(3) and eq (4) could lead to SD values in the range 0.4-0.5, and hence avoid the rather complicated similarity analysis, and to investigate if other indirect methods for estimating octanol solubility would result in similar, or better, statistics.

2. Results and discussion

As a starting point we use the same linear free energy relationship, eq. (7), that we have previously employed (Abraham, 1993; Abraham, Ibrahim and Zissimos, 2004; Abraham, Smith, Luchtefeld, Boorem, Luo, and Acree, Jr, 2010)

$$\text{Log } SP = c + e. E + s. S + a. A + b. B + v. V \quad (7)$$

In eq. (7), $\log SP$, the dependent variable, is a property of a series of solutes in a given system. In the present case SP will be the octanol solubility for a series of solutes. The independent variables in eq. (7) are descriptors of the solutes. In brief, E is the solute excess molar refractivity in units of

$(\text{cm}^3 \text{ mol}^{-1})/10$, S is the solute dipolarity / polarizability, A and B are the overall or summation hydrogen bond acidity and basicity and V is the McGowan volume in units of $(\text{cm}^3 \text{ mol}^{-1})/100$.

We first applied eq (7) to the data sets previously used (Admire and Yalkowsky, 2013; Raevsky, Perlovich and Schaper, 2007). In our previous work on solubility in water (Abraham and Le, 1999) we found that eq (7) gave disappointing results unless a descriptor ($A*B$) that dealt with solute-solute interactions within the bulk liquid or solid was included. Similarly, we now found that the inclusion of the descriptor ($A*B$) yielded much better correlations. The obtained equations for the Admire data set are given as eq. (8) and eq (9) and for the Raevsky data set are given as eq (10) and eq (11). The term $s \cdot S$ in Eqs. (8) and (9) was not statistically significant and was omitted. There is quite a difference between the coefficients in the Admire and the Raevsky equations. This is probably due to the two sets of compounds occupying somewhat different property spaces. Thus the average value of B in the Admire set is 0.65 and the average value in the Raevsky set is 0.80. The very useful statistic, PSD , the predicted standard deviation is obtained from the leave-one-out statistics as described before (Abraham, Acree, Jr., Leo and Hoekman, 2009)

$$\begin{aligned} \text{Log } S_{oct}(\text{mol/L}) &= 0.705 - 0.985 E + 0.465 A - 0.626 B + 0.335 V - 0.929 A*B \\ N &= 201, SD = 0.61, R^2 = 0.709, F = 95.0, Q^2 = 0.687, PSD = 0.63 \end{aligned} \quad (8)$$

$$\begin{aligned} \text{Log } S_{oct}(\text{mol/L}) &= 0.536 - 0.405E + 1.314A - 0.464B + 0.228V - 1.117A*B \\ &- 0.00764 (\text{mp-25}) \\ N &= 201, SD = 0.47, R^2 = 0.831, F = 157.8, Q^2 = 0.826, PSD = 0.49 \end{aligned} \quad (9)$$

$$\begin{aligned} \text{Log } S_{oct}(\text{mol/L}) &= -0.173 - 0.813 E - 0.439 S + 1.314 A - 0.402 B + 0.852 V \\ &- 1.524 A*B \\ N &= 170, SD = 0.61, R^2 = 0.689, F = 60.2, Q^2 = 0.678, PSD = 0.63 \end{aligned} \quad (10)$$

$$\begin{aligned} \text{Log } S_{oct}(\text{mol/L}) &= -0.140 - 0.377E - 0.464 S + 1.817 A - 0.280B + 0.686V - 1.601A*B \\ &- 0.00499 (\text{mp-25}) \\ N &= 170, SD = 0.54, R^2 = 0.761, F = 73.6, Q^2 = 0.715, PSD = 0.59 \end{aligned} \quad (11)$$

Finally, we combine the two data sets, together with some additional compounds taken from the literature (Alexander et al., 1977; Gharavi et al, 1983; Martin, Wu and Beerbower, 1984; Niimi,

1991; Pinsuwan, Li and Yalkowsky, 1995; Bernazzani et al., 1995; Kristl and Vesnaver, 1995; Bustamante, Pena and Barra, 1998; Martinez and Gomez, 2001; Avila and Martínez, 2002; Perlovich et al., 2003, 2010, 2011; Ran et al., 2002; Sepassi and Yalkowsky, 2006; Quingzhu et al., 2007, 2008; Thimmasetty et al, 2008) or from our own previous work (Fletcher et al., 1998; Hoover et al., 2004, 2005a, 2005b, 2006; Charlton et al., 2005; Stovall et al., 2005a, 2005b; Flanagan et al., 2006a, 2006b; Holley et al., 2011; Ye et al., 2011; Stephens et al., 2012; Wilson et al., 2012; Bowen et al., 2013). For most of the common compounds in the Admire and Raevsky data sets, the listed log *Soct*(mol/L) values were the same. In a few cases where they differed, we took the average. The resulting equations are given as eq (12) and eq (13); Mirex was a wild outlier to eq (13), though not to eq (12), and was excluded from both. The entire data set of compounds that we used is in Table 1, together with the compound descriptors.

Table 1 here

$$\text{Log } Soct(\text{mol/L}) = 0.604 - 0.942 E - 0.311 S + 0.588 A - 0.463 B + 0.540 V - 1.104 A*B \quad (12)$$

$$N = 282, SD = 0.63, R^2 = 0.691, F = 102.7, Q^2 = 0.672, PSD = 0.65$$

$$\text{Log } Soct(\text{mol/L}) = 0.480 - 0.355 E - 0.203 S + 1.521 A - 0.408 B + 0.364 V - 1.294 A*B - 0.00813 (\text{mp-25}) \quad (13)$$

$$N = 282, SD = 0.47, R^2 = 0.830, F = 190.9, Q^2 = 0.817, PSD = 0.48$$

For the Yalkowsky data set, the statistics for eq (9) are markedly better than those for eq (1), so that if the necessary descriptors are available, eq (9) is preferred. It is not so easy to compare eq (10) and eq (11) with equations given by Raevsky, because the preferred equations (Raevsky, Perlovich and Schaper, 2007) refer only to the best subset (158 compounds) out of the total of 218 compounds. Bearing this in mind, results from eq (10) and eq (11) are at least as good as those from the much more complicated similarity method (see Fig. 1).

For the combined (total) data set, both eq (12) and eq (13) yield quite good statistics, with SD = 0.63 and 0.47 log units respectively. If the experimental error in log *Soct*(mol/L) is indeed about 0.4 (Raevsky, Perlovich and Schaper, 2007) then the statistics of eq (13) might be as good as it is possible to get, without over-fitting the data. A recent survey of solubility in water (Hansen et al., 2006) leads to similar conclusions, with values of RMSE ranging from 0.46 log units from an

equation that uses 46 descriptors and an RSME of 0.47 log units from an equation with 33 descriptors to an RSME of 0.76 log units from an equation with 31 descriptors and an RSME of 0.98 log units from an equation with 4 descriptors.

We suggest that if the necessary descriptors are available then eq (13) is the preferred equation for estimations of $\log S_{oct}(\text{mol/L})$, with an SD of 0.47 log units. If the descriptors are not available, then eq. (1) will provide an estimate of $\log S_{oct}(\text{mol/L})$ with an SD of 0.71 log units (Admire and Yalkowsky, 2013). Both of these equations require a knowledge of the compound melting point. If this is not known, then eq. (5) with an SD of 0.66 log units or eq. (12) with an SD of 0.63 log units can be used. Eq. (12) is slightly the better statistically and seems less complicated than eq. (5) and so is preferred.

Although the SD value of 0.47 log units for eq. (13) is quite close to the expected experimental error of 0.4 log units, it is possible that other approaches to the estimation of $\log S_{oct}(\text{mol/L})$ values might lead to better predictive equations. A solubility ratio, SR , can be defined through eq (14) where S_{oct} and S_w are solubilities, in mol/L, in dry octanol and in water (Pinsuwan, Li and Yalkowsky, 1995). Values of SR were shown to be approximately correlated to the water-wet octanol partition coefficient, $P_{oct}(wet)$. However, a theoretically more satisfactory connection is between SR and the water-dry octanol partition coefficient, eq. (15). Then S_{oct} can be calculated through eq. (16).

$$SR = S_{oct} / S_w \quad (14)$$

$$SR = S_{oct} / S_w = P_{oct}(dry) \quad (15)$$

$$\log S_{oct}(\text{mol/L}) = \log P_{oct}(dry) + \log S_w(\text{mol/L}) \quad (16)$$

We have established (Abraham, Le, Acree, 1999) an equation for $\log P_{oct}(dry)$ and so can calculate the latter through eq (17). Then a knowledge of $\log S_w(\text{mol/L})$ enables $\log S_{oct}(\text{mol/L})$ to be estimated by another route. We had 228 compounds for which we had both terms on the right hand side of eq. (16), which yielded $\log S_{oct}(\text{mol/L})$ with an average error $AE = 0.02$ and $SD = 0.49$ log units. A plot of $\log S_{oct}(\text{mol/L})$ vs $[\log P_{oct}(dry) + \log S_w(\text{mol/L})]$ gave the coefficients shown in eq (18), with $N = 228$, $SD = 0.51$ and $PSD = 0.52$. The compound melting point is not used in eq. (18), but these equations have the disadvantage that the aqueous solubility is required, and so they offer no real advantage over eq. (13).

$$\text{Log } P_{oct}(dry) = -0.034 + 0.489 E - 1.044 S - 0.024 A - 4.235 B + 4.218 V \quad (17)$$

$$\text{Log } S_{oct}(\text{mol/L}) = -0.115 + 0.844 [\log P_{oct}(dry) + \log S_w(\text{mol/L})] \quad (18)$$

$$N = 228, SD = 0.51, R^2 = 0.799, F = 896.7, Q^2 = 0.795, PSD = 0.52$$

It is possible to interpret eq. (13) and, especially, eq. (12) in terms of the structural factors that influence solubility in dry octanol. However, it should be noted that solubility depends on two sets of interactions – those within the liquid or solid compound that will tend to reduce solubility, and those between the compound and the octanol solvent that will tend to increase solubility. It is useful to compare our equations for solubility in octanol with those for solubility in water (Le, 2001), eq. (19) and eq. (20).

$$\begin{aligned} \text{Log } S_{water}(\text{mol/L}) = & 0.394 - 0.954 E + 0.318 S + 1.157 A + 3.255 B - 3.329 V \\ & - 0.786 A*B \end{aligned} \quad (10)$$

$$N = 1071, SD = 0.67, R^2 = 0.888, F = 1401.0$$

$$\begin{aligned} \text{Log } S_{water}(\text{mol/L}) = & 0.368 - 0.711 E + 0.407 S + 1.730 A + 3.383 B - 3.493 V - 1.036 A*B \\ & - 0.0050 (\text{mp}-25) \end{aligned} \quad (20)$$

$$N = 944, SD = 0.61, R^2 = 908, F = 1324.0$$

The eE term in both eq. (12) and eq. (19) is negative, suggesting that dispersive interactions in the liquid or solid reduce solubility. The sS term is rather small in both eq. (12) and eq. (19); that in eq. (12) is negative so that dipole-dipole interactions in the liquid or solid are greater than dipole (solute) – dipole (octanol) interactions. Not surprisingly, dipole (solute) – dipole (water) interactions are much larger, leading to a positive sS term for solubility in water. The effect of compound hydrogen bond acidity is not straight forward, because increase in A increases solubility in both octanol and in water through the aA term, but decreases solubility through the $A*B$ term. The effect of hydrogen bond basicity is much clearer; solubility in water is greatly enhanced by increase in B , but solubility in octanol is slightly decreased. Water is a much stronger hydrogen bond acid than is octanol and so compound (base)-water (acid) interactions are dominant. The effect of compound volume is very interesting. Increase in volume slightly increases solubility in

octanol but greatly reduces solubility in water. These volume effects are resultants of general dispersion interactions that increase solubility in octanol (greatly) and increase solubility in water (to a less extent) and the work needed to create a cavity that decreases solubility in octanol (to a less extent) and decreases solubility in water (greatly).

3. Conclusions

The equations eq. (6) and eq. (13) for $\log S_{oct}(\text{mol/L})$ yield values of $SD = 0.46$ and 0.47 respectively. In view of the experimental error in $\log S_{oct}(\text{mol/L})$, of around 0.4 log units, these SD values are as low as is likely to be achieved without over-fitting of the data. The method of construction of eq. (13) is much simpler than that of eq. (6), and eq (13) is our recommended equation for the estimation of further values of solubility in dry octanol, as $\log S_{oct}(\text{mol/L})$. If the required descriptors in eq. (13) are not available, then the simple Yalkowsky equation, eq. (1), can be used although with a significantly higher SD value of 0.71 log units. All these equations require knowledge of a compound's melting point. If this is not known then eq. (12) with $SD = 0.63$ can be used. Other equations do not require a knowledge of melting point, but make use of solubility in water, and so are not likely to be as useful as eq. (13).

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Figure 1

Fig. 1. How the descriptors affect solubility in octanol.

1 Table 1.
2 The compounds used, their melting points, their solubility in dry octanol as log S/M, their descriptors, references for solubility in dry octanol, their solubility in water as log Sw
3 and their water-dry octanol partition coefficient as log *Poct*.
4

Compound	Tm/C	log S/M	<i>E</i>	<i>S</i>	<i>A</i>	<i>B</i>	<i>V</i>	<i>S</i> * <i>S</i>	<i>A</i> * <i>B</i>	mp-25	Ref	log <i>Sw</i>	log <i>Poct</i> dry	log <i>Poct</i> + log <i>Sw</i>
1,2,3,4-Tetrachloronaphthalene	198.0	-1.780	1.810	1.24	0.00	0.00	1.5750	1.5376	0.0000	173	a	-7.800	6.200	-1.600
1,2,3,5-Tetrachlorobenzene	51.5	0.150	1.160	0.85	0.00	0.00	1.2060	0.7225	0.0000	27	b,c	-4.732	4.733	0.001
1,2,3-Trichlorobenzene	53.0	0.150	1.030	0.86	0.00	0.00	1.0836	0.7396	0.0000	28	a	-4.089	4.142	0.053
1,2,4,5-Tetrabromobenzene	182.0	-1.260	1.830	1.19	0.00	0.00	1.4164	1.4161	0.0000	157	a	-6.980	5.593	-1.387
1,2,4,5-Tetrachlorobenzene	139.0	-1.000	1.160	0.86	0.00	0.00	1.2060	0.7396	0.0000	114	a	-5.316	4.722	-0.594
1,2,4,5-Tetramethylbenzene	79.0	-0.121	0.739	0.60	0.00	0.19	1.2800	0.3600	0.0000	54	d	-4.590	4.295	-0.295
1,2,4-Thiadiazole-1	102.0	-0.906	1.900	1.20	0.47	1.25	1.7479	1.4400	0.5875	77	e	-2.301	1.721	-0.580
1,2,4-Thiadiazole-2	117.0	-1.340	1.900	1.20	0.47	1.25	1.8888	1.4400	0.5875	92	e	-2.661	2.316	-0.345
1,2,4-Thiadiazole-3	112.0	-0.689	1.980	1.44	0.47	1.45	2.0884	2.0736	0.6815	87	e	-3.004	2.099	-0.905
1,2,4-Thiadiazole-4	103.0	-0.424	1.780	1.21	0.50	1.17	1.7656	1.4641	0.5850	78	f	-2.470	2.066	-0.404
1,2,4-Thiadiazole-5	144.0	-0.612	1.520	1.16	0.50	1.20	1.9419	1.3456	0.6000	119	f	-3.764	2.607	-1.157
1,2,4-Thiadiazole-6	145.0	-1.230	2.070	1.48	0.76	1.75	2.0884	2.1904	1.3300	120	f	-3.117	0.831	-2.286
1,2,4-Tribromobenzene	44.0	-0.110	1.450	1.07	0.00	0.00	1.2414	1.1449	0.0000	19	a	-4.500	4.794	0.294
1,2,4-Trichlorobenzene	25.0	0.551	0.980	0.81	0.00	0.00	1.0836	0.6561	0.0000	0	b	-3.610	4.170	0.560
1,2,5,6-Dibenzanthracene Dibenz[a,h]anthracene	266.0	-3.030	4.000	2.04	0.00	0.44	2.1924	4.1616	0.0000	241	b	-8.400	7.176	-1.224
1,2-Dichlorobenzene	25.0	0.568	0.872	0.78	0.00	0.04	0.9612	0.6084	0.0000	0	b	-3.020	3.463	0.443
1,2-Diphenylethane	51.5	-0.350	1.220	1.04	0.00	0.33	1.6060	1.0816	0.0000	27	b,c	-4.600	4.853	0.253
1,3,5-Tribromobenzene	122.0	-0.870	1.450	1.02	0.00	0.00	1.2414	1.0404	0.0000	97	a	-5.600	4.846	-0.754
1,3,5-Trichlorobenzene	64.0	-0.100	0.980	0.73	0.00	0.00	1.0836	0.5329	0.0000	39	a	-4.575	4.254	-0.321
1,3-Dibromobenzene	25.0	0.552	1.170	0.88	0.00	0.04	1.0664	0.7744	0.0000	0	b	-3.540	3.948	0.408
1,3-Dichlorobenzene	25.0	0.568	0.847	0.73	0.00	0.02	0.9612	0.5329	0.0000	0	b	-3.070	3.588	0.518
1,4-Dibromobenzene	88.0	-0.250	1.150	0.86	0.00	0.04	1.0664	0.7396	0.0000	63	a	-4.072	3.959	-0.113
1,4-Dichlorobenzene	55.0	0.170	0.825	0.75	0.00	0.02	0.9612	0.5625	0.0000	30	a	-3.329	3.556	0.227
17-alpha-Methyltestosterone	165.0	-0.587	1.490	2.57	0.29	1.25	2.5236	6.6049	0.3625	140	b	-3.970	3.362	-0.608
1-Chloroanthraquinone	159.0	-1.969	1.900	1.79	0.00	0.57	1.6512	3.2041	0.0000	134	d	-5.540	3.577	-1.963
1-Methoxy-2,3,4,5-tetrachlorobenzene	88.0	-0.560	1.280	1.15	0.00	0.08	1.4056	1.3225	0.0000	63	c		4.981	

1-Methoxy-2,3,4-trichlorobenzene	70.0	-0.420	1.130	1.18	0.00	0.10	1.2832	1.3924	0.0000	45	c		4.276	
1-Methylfluorene	85.0	-0.560	1.588	1.06	0.00	0.25	1.4974	1.1236	0.0000	60	b, c	-5.218	4.893	-0.325
1-Nitronaphthalene	62.0	-0.423	1.600	1.59	0.00	0.29	1.2596	2.5281	0.0000	37	d	-3.540	3.173	-0.367
2,3,4-Trichloroanisole	69.0	-0.360	1.130	1.18	0.00	0.10	1.2832	1.3924	0.0000	44	a		4.276	
2,3,4-Trichloronitrobenzene	55.5	-0.270	1.319	1.40	0.00	0.15	1.2578	1.9600	0.0000	31	a	-3.939	3.820	-0.119
2,3,4,5-Tetrachloroanisole	84.0	-0.520	1.280	1.15	0.00	0.08	1.4056	1.3225	0.0000	59	a		4.981	
2,3,5,6-Tetrachloronitrobenzene	99.5	-0.630	1.465	1.43	0.00	0.09	1.3802	2.0449	0.0000	75	b,c	-5.097	4.630	-0.467
2,3-Benzanthracene, Naphthacene	341.0	-2.280	2.847	1.70	0.00	0.29	1.8234	2.8900	0.0000	316	g	-8.190	6.046	-2.144
2,3-Benzofluorene Benzo[b]fluorene	210.0	-1.750	2.622	1.57	0.00	0.24	1.7255	2.4649	0.0000	185	b,c	-7.740	5.871	-1.869
2,4,5-Trichlorotoluene	82.4	-0.390	1.060	0.86	0.00	0.00	1.2245	0.7396	0.0000	57	a		4.751	
2,4,6-Trichlorophenol	65.0	0.250	1.010	0.80	0.60	0.15	1.1423	0.6400	0.0900	40	a	-2.341	3.808	1.467
2,4'-DDT	75.0	-0.420	1.850	1.70	0.00	0.25	2.2180	2.8900	0.0000	50	a	-6.620	7.393	0.773
2,4-Dichlorophenol	42.5	0.350	0.960	0.82	0.54	0.17	1.0199	0.6724	0.0918	18	a	-1.559	3.161	1.602
2,5-Dihydroxybenzoic acid	205.0	-0.130	1.140	1.33	1.14	0.64	1.0491	1.7689	0.7296	180	b,c		0.850	
2-Aminobenzoic acid	144.0	-0.416	1.075	1.48	0.74	0.50	1.0315	2.1904	0.3700	119	h	-1.600	1.180	-0.420
2-Bromobenzoic acid	149.0	-0.120	1.000	1.00	0.64	0.53	1.1067	1.0000	0.3392	124	b,c	-2.276	1.835	-0.441
2-Chlorobenzoic acid	140.0	-0.153	0.840	1.01	0.68	0.40	1.0541	1.0201	0.2720	115	b, h	-1.900	2.075	0.175
2-Ethylanthraquinone	109.0	-1.160	1.410	1.54	0.00	0.55	1.8106	2.3716	0.0000	84	d	-5.530	4.356	-1.174
2-Methylbenzoic acid	108.0	-0.003	0.730	0.84	0.42	0.44	1.0726	0.7056	0.1848	83	i	-2.060	2.107	0.047
2-Methyl-3,5-dinitrobenzoic acid	206.0	-1.103	1.310	2.12	0.75	0.65	1.4210	4.4944	0.4875	181	d	-2.600	1.634	-0.966
2-Nitrobenzoic acid	146.0	-0.318	0.990	1.48	0.82	0.53	1.1059	2.1904	0.4346	121	i	-1.330	1.325	-0.005
3,4-Dichloronitrobenzene	41.3	-0.020	1.168	1.22	0.00	0.19	1.1354	1.4884	0.0000	16	a	-3.201	3.248	0.047
3,4-Dichlorosulfabenzene	224.8	-2.570	0.890	1.57	0.58	0.76	1.3309	2.4649	0.4408	200	c		1.157	
3,4-Dimethoxybenzoic acid	181.0	-1.410	0.950	1.65	0.57	0.75	1.3309	2.7225	0.4275	156	d	-2.510	1.145	-1.365
3-Bromobenzoic acid	157.0	-0.070	1.000	1.10	0.64	0.27	1.1067	1.2100	0.1728	132	b,c	-2.699	2.831	0.132
3-Methoxybenzoic acid	106.0	-1.080	0.830	0.90	0.62	0.55	1.1313	0.8100	0.3410	81	b		1.875	
3-Methylbenzoic acid	110.0	0.057	0.730	0.89	0.60	0.40	1.0726	0.7921	0.2400	85	i		2.224	
3-Nitrobenzoic Acid	141.0	-0.026	0.990	1.18	0.73	0.52	1.1059	1.3924	0.3796	116	d	-1.680	1.681	0.001
3,4-Dichlorobenzoic acid	208.0	-0.814	0.950	0.92	0.67	0.26	1.1766	0.8464	0.1742	183	d	-3.980	3.332	-0.648
4,4'-DDE	89.0	-0.680	1.800	1.40	0.06	0.14	2.0526	1.9600	0.0084	64	a	-6.420	7.450	1.030
4,4'-DDT	110.0	-0.460	1.805	1.76	0.00	0.16	2.2180	3.0976	0.0000	85	a, b	-7.512	7.689	0.177

4-Acetylaminophenol Paracetamol	170.0	-0.815	1.120	1.63	1.01	0.91	1.1724	2.6569	0.9191	145	b,c	-1.030	-0.097	-1.127
4-Aminobenzoic acid	189.0	-0.800	1.075	1.65	0.94	0.60	1.0315	2.7225	0.5640	164	c	-1.350	0.579	-0.771
4-Bromoaniline	66.0	0.430	1.190	1.19	0.31	0.30	0.9912	1.4161	0.0930	41	j		2.216	
4-Bromobenzoic acid	253.0	-1.110	1.000	1.01	0.63	0.26	1.1067	1.0201	0.1638	228	b, c	-3.539	2.968	-0.571
4-Chloronitrobenzene	83.5	-0.280	0.980	1.22	0.00	0.24	1.0130	1.4884	0.0000	59	b,c	-2.920	2.428	-0.492
4-Hydroxybenzoic acid	216.0	-0.179	0.930	0.90	0.81	0.56	0.9904	0.8100	0.4536	191	i	-1.400	1.287	-0.113
4-Methylbenzoic acid	181.0	-0.320	0.730	0.93	0.63	0.44	1.0726	0.8649	0.2772	156	b, i	-2.562	2.013	-0.549
4-Nitrobenzoic acid	240.0	-1.209	0.990	0.52	0.68	0.40	1.1059	0.2704	0.2720	215	d	-2.980	2.878	-0.102
5-Amino-o-cresol	161.0	-0.760	1.100	1.16	0.65	0.76	1.0158	1.3456	0.4940	136	j		0.359	
5-Fluorouracil	283.0	-2.340	0.720	0.84	0.57	1.02	0.7693	0.7056	0.5814	258	c	-1.070	-1.634	-2.704
6-Deoxyacyclovir	188.0	-3.040	2.190	2.40	0.45	1.58	1.4630	5.7600	0.7110	163	b,c	-1.080	-1.989	-3.069
6-Mercaptopurine	314.0	-2.820	1.750	1.70	0.40	1.00	0.9866	2.8900	0.4000	289	c		-1.027	
9-Fluorenone	83.0	-0.367	1.600	1.49	0.00	0.35	1.3722	2.2201	0.0000	58	d	-4.030	3.499	-0.531
9-Methylantracene	78.0	-0.600	2.250	1.27	0.00	0.30	1.5953	1.6129	0.0000	53	b,c	-5.870	5.199	-0.671
17a-Methyltestosterone	163.0	-0.599	1.490	2.57	0.20	1.25	2.5236	6.6049	0.2500	138	k	-3.850	3.362	-0.488
Acenaphthene	95.0	-0.590	1.604	1.05	0.00	0.22	1.2586	1.1025	0.0000	70	b,c	-4.615	4.031	-0.584
Acetanilide	114.0	-0.150	0.900	1.37	0.48	0.67	1.1137	1.8769	0.3216	89	b,c	-1.310	0.836	-0.474
Acetic acid	25.0	0.936	0.265	0.64	0.62	0.44	0.4648	0.4096	0.2728	0	b		-0.475	
Acetone	25.0	0.836	0.179	0.70	0.04	0.49	0.5470	0.4900	0.0196	0	b		-0.445	
Acetonitrile	25.0	0.983	0.237	0.90	0.07	0.32	0.4042	0.8100	0.0224	0	b	0.260	-0.508	-0.248
Acetylsalicylic acid	135.0	-0.690	0.781	1.69	0.71	0.67	1.2879	2.8561	0.4757	110	b, c	-1.614	1.178	-0.436
a-hexachlorocyclohexane	159.0	-1.190	1.450	0.73	0.00	0.71	1.5798	0.5329	0.0000	134	a	-5.160	3.570	-1.590
Alclofenac	92.0	-0.215	1.060	1.48	0.56	0.80	1.6334	2.1904	0.4480	67	b	-3.130	2.441	-0.689
Aminopyrine	107.8	0.000	1.680	1.74	0.00	1.60	1.8662	3.0276	0.0000	83	b,c	-0.629	0.067	-0.562
Anthracene	216.3	-1.780	2.290	1.34	0.00	0.28	1.4544	1.7956	0.0000	191	g	-6.107	4.636	-1.471
Antipyrine	112.3	-0.190	1.300	1.83	0.00	1.37	1.4846	3.3489	0.0000	87	b,c	-0.559	-0.849	-1.408
Atenolol	146.0	-1.909	1.450	1.90	0.62	2.03	2.1763	3.6100	1.2586	121	b		-0.726	
Atrazine	177.0	-1.320	1.220	1.29	0.17	1.01	1.6196	1.6641	0.1717	152	b,c	-3.866	1.770	-2.096
Barbital	190.0	-0.920	1.030	1.00	0.58	1.12	1.3739	1.0000	0.6496	165	b,c	-1.430	0.478	-0.952
Barbituric acid	248.0	-0.920	1.090	1.19	0.49	1.16	0.8103	1.4161	0.5684	223	b,c	0.930	-2.238	-1.308
Benzene	25.0	0.750	0.610	0.52	0.00	0.14	0.7164	0.2704	0.0000	0	b	-1.640	2.150	0.510

Benzil	95.0	-0.890	1.445	1.59	0.00	0.62	1.6374	2.5281	0.0000	70	g		3.293	
Benzo[a]pyrene	176.0	-1.550	3.625	1.96	0.00	0.37	1.9536	3.8416	0.0000	151	a	-8.699	6.366	-2.333
Benzoic acid	122.0	-0.060	0.730	0.90	0.59	0.40	0.9317	0.8100	0.2360	97	b,c	-1.560	1.619	0.059
Benzoin	137.0	-1.736	1.585	2.11	0.20	0.85	1.6804	4.4521	0.1700	112	d	-3.670	2.026	-1.644
Benzocaine, Ethyl 4-aminobenzoate	90.0	-0.400	1.030	1.31	0.31	0.69	1.3133	1.7161	0.2139	65	l	-2.237	1.719	-0.518
Ethyl 4-aminobenzoate	89.0	-0.310	1.030	1.31	0.31	0.69	1.3133	1.7161	0.2139	64	b,c	-2.237	1.719	-0.518
Benzyl Alcohol	25.0	0.682	0.803	0.87	0.39	0.56	0.9160	0.7569	0.2184	0	b	-0.432	0.942	0.510
Bifonazole	142.0	-1.454	2.410	2.13	0.00	1.15	2.5006	4.5369	0.0000	117	b		4.598	
Bibenzyl	52.0	-0.350	1.220	0.93	0.00	0.33	1.6060	0.8649	0.0000	27	g	-4.627	4.968	0.341
Biphenyl	69.0	-0.130	1.360	0.99	0.00	0.26	1.3242	0.9801	0.0000	44	b,c	-4.139	4.082	-0.057
Butane	25.0	0.695	0.000	0.00	0.00	0.00	0.6722	0.0000	0.0000	0	b	-2.950	2.801	-0.149
Butanol	25.0	0.740	0.224	0.42	0.37	0.48	0.7309	0.1764	0.1776	0	b	0.000	0.687	0.687
Butyl 4-aminobenzoate	58.0	0.130	1.010	1.35	0.30	0.68	1.5951	1.8225	0.2040	33	b,c	-2.100	2.899	0.799
Butyl 4-hydroxybenzoate	69.0	0.254	0.900	1.47	0.74	0.43	1.5540	2.1609	0.3182	44	m	-3.320	3.605	0.285
Caffeine	236.0	-1.720	1.500	1.82	0.08	1.25	1.3632	3.3124	0.1000	211	b,c	-0.086	-0.744	-0.830
Carbazole	247.0	-1.290	1.787	1.82	0.22	0.18	1.3154	3.3124	0.0396	222	b,c	-5.270	3.726	-1.544
Carbon tetrachloride	25.0	0.717	0.458	0.38	0.00	0.00	0.7391	0.1444	0.0000	0	b	-2.300	2.911	0.611
Cholesterol	148.0	-0.472	1.360	1.35	0.32	0.85	3.4942	1.8225	0.2720	123	b		10.360	
Chrysene	255.0	-2.530	3.027	1.73	0.00	0.36	1.8234	2.9929	0.0000	230	a	-7.857	5.807	-2.050
a-Chlordane, cis-Chlordane	106.0	-0.650	2.100	1.27	0.00	0.50	2.1280	1.6129	0.0000	81	a	-6.860	6.525	-0.335
b-Chlordane, trans-Chlordane	104.0	-0.390	2.100	1.46	0.00	0.45	2.1280	2.1316	0.0000	79	a	-6.860	6.539	-0.321
Coronene	438.0	-3.410	4.236	1.99	0.00	0.55	2.2140	3.9601	0.0000	413	g		6.969	
Cortisone	225.0	-1.970	1.960	3.50	0.36	1.87	2.7546	12.2500	0.6732	200	b,c	-3.120	0.970	-2.150
Cyclohexane	25.0	0.666	0.305	0.10	0.00	0.00	0.8454	0.0100	0.0000	0	b	-3.200	3.577	0.377
Dichloromethane	25.0	0.886	0.387	0.57	0.10	0.05	0.4943	0.3249	0.0050	0	b	-0.800	1.433	0.633
Dimetridazole	140.0	-1.100	0.920	1.65	0.00	0.68	0.9923	2.7225	0.0000	115	g			
Deoxycorticosterone	142.0	-0.710	1.740	3.50	0.14	1.31	2.6802	12.2500	0.1834	117	b,c	-3.450	2.920	-0.530
Diazepam	130.0	-1.010	2.170	1.78	0.00	1.27	2.0739	3.1684	0.0000	105	b,c	-3.750	2.538	-1.212
Dibenz[ah]anthracene	269.0	-3.030	4.000	2.04	0.00	0.44	2.1924	4.1616	0.0000	244	b,c	-8.740	7.176	-1.564
Dibenzofuran	82.0	-0.270	1.407	1.13	0.00	0.17	1.2743	1.2769	0.0000	57	g	-4.700	4.129	-0.571
Diclofenac	157.0	-1.110	1.810	1.85	0.55	0.77	2.0250	3.4225	0.4235	132	b,c	-5.100	4.200	-0.900

Dieldrin	175.0	-0.940	2.090	1.46	0.00	0.65	2.0065	2.1316	0.0000	150	a	-6.248	5.174	-1.074
Diphenylamine	53.0	0.030	1.470	1.13	0.31	0.31	1.4240	1.2769	0.0961	28	b,c	-3.504	4.199	0.695
Diuron	159.0	-1.140	1.280	1.60	0.57	0.70	1.5992	2.5600	0.3990	134	b,c	-4.025	2.702	-1.323
DMSO	25.0	0.836	0.522	1.72	0.00	0.97	0.6126	2.9584	0.0000	0	b		-3.098	
Endrin	210.0	-0.920	2.090	1.57	0.00	0.75	2.0065	2.4649	0.0000	185	a	-6.174	4.636	-1.538
Estradiol	176.0	-0.990	1.800	1.77	0.86	1.10	2.1988	3.1329	0.9460	151	b,c	-4.850	3.614	-1.236
Ethanol	25.0	0.936	0.246	0.42	0.37	0.48	0.4491	0.1764	0.1776	0	b	1.100	-0.491	0.609
Ether (Diethylether)	25.0	0.678	0.041	0.25	0.00	0.45	0.7309	0.0625	0.0000	0	b	-0.090	0.902	0.812
Ethyl 4-hydroxybenzoate	116.0	-0.025	0.910	1.44	0.73	0.45	1.2722	2.0736	0.3285	91	m	-2.350	2.368	0.018
Ethyl acetate	25.0	0.703	0.106	0.62	0.00	0.45	0.7466	0.3844	0.0000	0	b	-0.040	0.614	0.574
Ethylene glycol	25.0	0.951	0.404	0.90	0.58	0.78	0.5078	0.8100	0.4524	0	b	1.060	-1.937	-0.877
Fenbufen	186.0	-1.920	1.780	1.80	0.62	1.05	1.9779	3.2400	0.6510	161	b,c	-5.060	2.853	-2.207
Fenchlorphos	38.0	-0.160	1.550	1.07	0.00	0.56	1.9096	1.1449	0.0000	13	b,c	-5.729	5.290	-0.439
Fentiazac	161.0	-0.770	2.356	2.06	0.67	0.82	2.2942	4.2436	0.5494	136	b	-4.960	5.172	0.212
Fenuron	132.0	-0.770	1.050	1.59	0.41	0.90	1.3544	2.5281	0.3690	107	b,c	-1.647	0.721	-0.926
Flufenamic Acid	125.0	-0.264	1.370	1.29	0.72	0.40	1.8333	1.6641	0.2880	100	b	-4.620	5.328	0.708
Fluoranthene	108.0	-0.760	2.377	1.55	0.00	0.24	1.5846	2.4025	0.0000	83	b,c	-5.915	5.178	-0.737
Fluorene	116.0	-0.620	1.588	1.06	0.00	0.25	1.3565	1.1236	0.0000	91	b,c	-4.885	4.299	-0.586
Fluorodifen	90.0	-1.520	1.344	2.06	0.00	0.65	1.9253	4.2436	0.0000	65	b,c	-5.215	3.841	-1.374
Flurbiprofen	114.0	-0.200	1.440	1.45	0.62	0.76	1.8389	2.1025	0.4712	89	b,c	-3.740	3.694	-0.046
Fumaric Acid	287.0	-1.120	0.710	0.94	0.87	0.59	0.7780	0.8836	0.5133	262	b,c	-1.279	0.115	-1.164
Furosemide	206.0	-2.090	2.306	2.19	1.03	1.50	2.1032	4.7961	1.5450	181	b	-3.660	1.326	-2.334
Gentisic acid	205.0	-0.130	1.140	1.33	1.14	0.64	1.0491	1.7689	0.7296	180	g	-1.759	0.850	-0.909
Griseofulvin	220.0	-2.470	1.750	2.64	0.00	1.44	2.3947	6.9696	0.0000	195	b,c	-4.600	2.068	-2.532
Heptachlor	95.0	-0.590	2.082	0.85	0.00	0.56	1.9626	0.7225	0.0000	70	a	-6.317	6.003	-0.314
Heptachlor epoxide	160.0	-0.910	2.215	1.11	0.00	0.53	1.9557	1.2321	0.0000	135	a	-6.050	5.895	-0.155
Hexabromobenzene	306.0	-2.620	2.530	1.52	0.00	0.00	1.7664	2.3104	0.0000	281	a	-9.700	7.067	-2.630
Hexachlorobenzene	230.0	-1.800	1.490	0.99	0.00	0.00	1.4508	0.9801	0.0000	205	a	-7.685	5.781	-1.904
Hexachlorobutadiene	25.0	0.500	1.019	0.42	0.00	0.16	1.3206	0.1764	0.0000	0	b	-4.910	4.919	0.009
Hexachloroethane	192.0	-0.230	0.680	0.68	0.00	0.00	1.1248	0.4624	0.0000	167	a	-4.488	4.333	-0.155
Hexadecane	25.0	0.582	0.000	0.00	0.00	0.00	2.3630	0.0000	0.0000	0	b	-8.400	9.933	1.533

Hexamethylbenzene	167.0	-0.890	0.950	0.72	0.00	0.28	1.5618	0.5184	0.0000	142	b,c	-5.277	5.081	-0.196
Hexane	25.0	0.585	0.000	0.00	0.00	0.00	0.9540	0.0000	0.0000	0	b	-4.000	3.990	-0.010
Hydrocortisone	218.0	-1.800	2.030	3.49	0.71	1.90	2.7976	12.1801	1.3490	193	b,c	-3.080	1.069	-2.011
Ibuprofen	76.0	0.070	0.730	0.70	0.57	0.79	1.7771	0.4900	0.4503	51	d	-3.760	3.742	-0.018
Indole-3-acetic acid	168.5	-0.590	1.510	1.70	0.88	0.79	1.3026	2.8900	0.6952	144	b,c		1.078	
Indomethacin	159.0	-1.470	2.240	1.47	0.58	1.43	2.5299	2.1609	0.8294	134	b,c	-4.620	4.142	-0.478
Indomethacin ethyl ester	96.0	-1.860	2.340	2.35	0.00	1.32	2.8117	5.5225	0.0000	71	c		4.926	
Iprnidazole	61.0	-0.060	0.900	1.59	0.00	0.78	1.2741	2.5281	0.0000	36	g		0.817	
Isazophos	25.0	0.500	1.520	1.45	0.00	1.31	2.1481	2.1025	0.0000	0	g	-3.321	2.708	-0.613
Isopropyl myristate	25.0	0.195	-0.062	0.53	0.00	0.45	2.5783	0.2809	0.0000	0	b		8.352	
Ketoprofen	93.0	-0.388	1.650	2.26	0.55	0.89	1.9779	5.1076	0.4895	68	n	-3.698	2.987	-0.711
Levonorgestrel	236.0	-1.830	1.900	2.54	0.45	1.40	2.5785	6.4516	0.6300	211	b		3.190	
Lindane	114.0	-0.660	1.450	0.91	0.00	0.68	1.5798	0.8281	0.0000	89	a	-4.464	3.509	-0.955
Lovastatin	175.0	-1.965	1.290	2.73	0.31	1.76	3.2859	7.4529	0.5456	150	b		4.153	
Mestanolone	192.0	-1.011	1.580	2.49	0.16	1.18	2.5666	6.2001	0.1888	167	k	-4.920	3.968	-0.952
Metalaxyl	72.0	-0.330	1.060	1.41	0.00	1.73	2.3153	1.9881	0.0000	47	c		1.452	
Methanediene	163.0	-0.459	1.450	2.37	0.31	1.12	2.4806	5.6169	0.3472	138	k	-4.280	3.921	-0.359
Methanol	25.0	1.097	0.278	0.44	0.43	0.47	0.3082	0.1936	0.2021	0	b		-1.048	
Methyl 4-aminobenzoate	114.0	-0.530	1.030	1.25	0.30	0.72	1.1724	1.5625	0.2160	89	b,c	-1.600	1.061	-0.539
Methyl 4-hydroxybenzoate	131.0	-0.070	0.930	1.46	0.71	0.46	1.1313	2.1316	0.3266	106	o	-1.826	1.720	-0.106
Metalaxyl	72.0	-0.330	1.060	1.41	0.00	1.73	2.3153	1.9881	0.0000	47	g	-1.601	1.452	-0.149
Metolachlor	25.0	0.470	1.113	1.53	0.00	1.25	2.2811	2.3409	0.0000	0	g	-2.729	3.241	0.512
Metoxuron	127.0	-1.060	1.240	1.78	0.32	1.07	1.6764	3.1684	0.3424	102	b,c	-2.581	1.254	-1.327
Monuron	174.0	-1.040	1.140	1.50	0.47	0.78	1.4768	2.2500	0.3666	149	b,c	-2.997	1.883	-1.114
Acyclovir	255.0	-3.960	1.900	1.88	0.82	1.88	1.5217	3.5344	1.5416	230	p	-2.146	-2.611	-4.757
6-Deoxyacyclovir	189.0	-3.041	2.190	2.40	0.45	1.58	1.4630	5.7600	0.7110	164	p	-1.078	-1.989	-3.067
N,O-Diacetyl-6-deoxyacyclovir	134.0	-2.632	2.050	2.96	0.41	2.02	2.0580	8.7616	0.8282	109	p	-0.728	-1.996	-2.724
N,O-Diacetylacyclovir	204.0	-3.796	2.290	2.48	0.64	2.23	2.1167	6.1504	1.4272	179	p	-2.143	-2.019	-4.162
N-Acetyl-6-deoxyacyclovir	181.0	-3.244	2.150	2.79	0.64	1.85	1.7605	7.7841	1.1840	156	p	-0.863	-2.304	-3.167
N-Acetylacyclovir	217.0	-4.027	2.420	2.20	0.87	2.13	1.8192	4.8400	1.8531	192	p	-1.923	-2.495	-4.418
O-Acetyl-6-deoxyacyclovir	135.0	-2.367	2.050	2.66	0.23	1.66	1.7605	7.0756	0.3818	110	p	-0.967	-1.413	-2.380

O-Acetylacyclovir	242.0	-4.920	2.300	2.12	0.60	2.06	1.8192	4.4944	1.2360	217	p	-2.670	-2.173	-4.843
Nadolol	124.0	-2.327	1.630	1.64	0.85	2.34	2.4923	2.6896	1.9890	99	b	-1.010	-0.346	-1.356
Nandrolone	112.0	-0.329	1.540	2.59	0.32	1.19	2.2418	6.7081	0.3808	87	k	-2.540	2.431	-0.109
Naphthacene	357.0	-2.270	2.847	1.70	0.00	0.29	1.8234	2.8900	0.0000	332	b,c	-8.190	6.046	-2.144
Naphthalene	82.0	-0.360	1.340	0.92	0.00	0.20	1.0854	0.8464	0.0000	57	a	-3.620	3.392	-0.228
Naproxen	155.0	-0.890	1.510	2.02	0.60	0.67	1.7821	4.0804	0.4020	130	b,c	-4.202	3.275	-0.927
Naproxen butyl ester	67.0	-0.880	1.430	1.63	0.00	0.89	2.3457	2.6569	0.0000	42	b,c		5.089	
Naproxen d-sec-butyl ester	45.0	-0.280	1.430	1.60	0.00	0.89	2.3457	2.5600	0.0000	20	b,c		5.120	
Naproxen ethyl ester	75.0	-0.700	1.430	1.62	0.00	0.89	2.0639	2.6244	0.0000	50	b,c		3.910	
Naproxen hexyl ester	42.0	-0.020	1.420	1.64	0.00	0.89	2.6275	2.6896	0.0000	17	b,c		6.262	
Naproxen isopropyl ester	64.0	-0.460	1.430	1.60	0.00	0.89	2.2048	2.5600	0.0000	39	b,c		4.526	
Naproxen tert-butyl ester	93.0	-1.040	1.410	1.57	0.00	0.89	2.3457	2.4649	0.0000	68	b,c		5.141	
Naproxol	87.0	-0.540	1.590	1.43	0.31	0.85	1.7664	2.0449	0.2635	62	b,c		3.102	
Naproxol acetate	61.0	-0.470	1.430	1.70	0.00	0.89	2.0639	2.8900	0.0000	36	b,c		3.827	
Nicotinic acid	236.6	-1.560	0.880	1.03	0.86	0.65	0.8906	1.0609	0.5590	212	b,c	-2.080	0.325	-1.755
Nifedipine	173.0	-1.560	1.503	2.45	0.23	1.45	2.4945	6.0025	0.3335	148	b,c	-4.760	2.524	-2.236
Niflumic Acid	204.0	-0.902	1.540	1.71	0.75	0.79	1.7922	2.9241	0.5925	179	b	-4.170	3.148	-1.022
Nitrobenzene	25.0	0.690	0.871	1.11	0.00	0.28	0.8906	1.2321	0.0000	0	b	-1.800	1.804	0.004
Nitrofurantoin	268.0	-3.360	2.295	2.36	0.24	1.42	1.4533	5.5696	0.3408	243	b	-3.480	-1.259	-4.739
N-Methylthalidomide	159.0	-2.010	1.982	2.43	0.00	1.28	1.8888	5.9049	0.0000	134	b,c		0.944	
N-Pentylthalidomide	105.0	-1.210	1.868	2.44	0.00	1.26	2.4524	5.9536	0.0000	80	b,c		3.340	
N-Propylthalidomide	136.0	-1.680	1.894	2.45	0.00	1.28	2.1706	6.0025	0.0000	111	b,c		2.069	
Octane	25.0	0.489	0.000	0.00	0.00	0.00	1.2358	0.0000	0.0000	0	b	-5.240	5.179	-0.061
Octachlorostyrene	95.0	-0.620	1.800	1.15	0.00	0.00	1.9344	1.3225	0.0000	70	a	7.390		
PCB-3	78.0	-0.220	1.500	1.05	0.00	0.18	1.4466	1.1025	0.0000	53	c	-5.200	4.943	-0.257
PCB-8	44.0	0.100	1.620	1.20	0.00	0.18	1.5690	1.4400	0.0000	19	b	-5.074	5.361	0.287
PCB-15	149.0	-0.850	1.640	1.18	0.00	0.16	1.5690	1.3924	0.0000	124	a	-6.445	5.476	-0.969
PCB-28	58.0	-0.130	1.760	1.33	0.00	0.15	1.6914	1.7689	0.0000	33	b	-6.481	5.937	-0.544
PCB-29, 2,4,5-Trichlorobiphenyl	78.0	-0.345	1.770	1.33	0.00	0.17	1.6914	1.7689	0.0000	53	b	-6.447	5.857	-0.590
PCB-31	65.0	-0.050	1.770	1.33	0.00	0.15	1.6914	1.7689	0.0000	40	b	-6.250	5.942	-0.308
PCB-52, 2,2',5,5'-Tetrachlorobiphenyl	87.0	-0.500	1.900	1.48	0.00	0.15	1.8138	2.1904	0.0000	62	b,c	-6.443	6.365	-0.078

PCB-61, 2,3,4,5-Tetrachlorobiphenyl	91.0	-0.440	1.920	1.46	0.00	0.13	1.8138	2.1316	0.0000	66	b	-7.261	6.481	-0.780
PBC-101	77.0	-0.230	2.040	1.61	0.00	0.13	1.9362	2.5921	0.0000	52	b	-7.022	6.899	-0.123
PCB-105	117.0	0.180	2.040	1.59	0.00	0.11	1.9362	2.5281	0.0000	92	b	-7.670	7.005	-0.665
PCB-118	110.0	-0.010	2.060	1.59	0.00	0.11	1.9362	2.5281	0.0000	85	b	-7.390	7.014	-0.376
PCB-138	79.0	0.000	2.180	1.74	0.00	0.11	2.0586	3.0276	0.0000	54	b	-8.410	7.433	-0.977
PCB-153	103.0	-0.210	2.180	1.74	0.00	0.11	2.0586	3.0276	0.0000	78	b	-8.443	7.433	-1.010
PCB-155	113.0	-0.220	2.120	1.74	0.00	0.11	2.0586	3.0276	0.0000	88	b	-8.598	7.403	-1.195
PCB-180	112.0	-0.110	2.290	1.87	0.00	0.09	2.1810	3.4969	0.0000	87	b	-9.500	7.952	-1.548
PCB-194	157.0	0.070	2.480	2.00	0.00	0.06	2.3034	4.0000	0.0000	132	b	-8.487	8.552	0.065
PCB-209, Decachlorobiphenyl	306.0	-2.770	2.720	2.26	0.00	0.02	2.5482	5.1076	0.0000	281	b, g	-11.620	9.600	-2.020
Pentachlorobenzene	85.0	-0.560	1.330	0.92	0.06	0.00	1.3284	0.8464	0.0000	60	b,c	-5.493	5.259	-0.234
Pentachloronitrobenzene	144.0	-0.980	1.610	1.46	0.00	0.02	1.5026	2.1316	0.0000	119	b,c	-5.800	5.482	-0.318
Pentachlorophenol	189.5	-0.130	1.220	0.86	0.64	0.08	1.3871	0.7396	0.0512	165	a	-4.290	5.177	0.887
Pentachlorotoluene	224.8	-1.560	1.390	1.00	0.00	0.00	1.4693	1.0000	0.0000	200	a		5.799	
Pentazocin	146.0	-0.590	1.400	1.15	0.60	1.25	2.4464	1.3225	0.7500	121	c		4.475	
Perylene	278.0	-2.520	3.256	1.76	0.00	0.42	1.9536	3.0976	0.0000	253	b,c	-8.798	6.182	-2.616
Phenacetin	135.0	-0.840	0.940	1.48	0.48	0.86	1.4542	2.1904	0.4128	110	b,c	-2.350	1.372	-0.978
Phenanthrene	101.0	-0.490	2.055	1.29	0.00	0.29	1.4544	1.6641	0.0000	76	a	-5.219	4.531	-0.688
Phenobarbital	176.0	-1.090	1.630	1.72	0.71	1.18	1.6999	2.9584	0.8378	151	b,c	-2.340	1.140	-1.200
Phenol	41.0	0.940	0.805	0.89	0.60	0.30	0.7751	0.7921	0.1800	16	b,c	-0.009	1.429	1.420
Phenothazine	187.0	-0.931	1.890	1.56	0.31	0.30	1.4789	2.4336	0.0930	162	d	-5.100	4.229	-0.871
Phenylbutazone	107.0	-1.634	2.281	2.25	0.00	1.30	2.4329	5.0625	0.0000	82	b	-3.810	3.489	-0.321
Pimozide	216.0	-1.590	2.508	2.54	0.33	1.70	3.4743	6.4719	0.5617	191	q	-7.650	5.983	-1.667
Piroxicam	198.0	-2.723	2.560	2.76	0.70	1.55	2.2500	7.6176	1.0850	173	d	-4.160	1.263	-2.897
Prednisolone	240.0	-1.620	2.210	3.10	0.71	1.92	2.7546	9.6100	1.3632	215	b,c	-3.100	1.298	-1.802
Profluralin	32.0	-0.200	1.210	1.67	0.00	0.57	2.2363	2.7889	0.0000	7	b,c	-6.541	5.833	-0.708
Progesterone	130.0	-0.710	1.450	3.29	0.00	1.14	2.6215	10.8241	0.0000	105	b,c	-4.449	3.470	-0.979
Propanol	25.0	0.824	0.236	0.42	0.37	0.48	0.5900	0.1764	0.1776	0	b	0.620	0.099	0.719
Propyl 4-hydroxybenzoate	96.0	0.069	0.900	1.45	0.74	0.43	1.4131	2.1025	0.3182	71	m	-2.600	3.032	0.432
Propylene glycol	25.0	0.830	0.373	0.90	0.58	0.80	0.6487	0.8100	0.4640	0	b		-1.443	
p-Xylene	25.0	0.609	0.613	0.52	0.00	0.16	0.9982	0.2704	0.0000	0	b	-2.770	3.256	0.486

Pyrene	151.0	-0.920	2.808	1.71	0.00	0.28	1.5846	2.9241	0.0000	126	a	-6.235	5.052	-1.183
S6,9-Bis(acetyloxymethyl)-6-mercaptopurine	121.5	-2.140	1.900	2.50	0.00	1.64	1.9808	6.2500	0.0000	97	c		-0.305	
S6,9-Bis(butanoyloxymethyl)-6-mercaptopurine	69.0	-1.120	1.900	2.50	0.00	1.65	2.5444	6.2500	0.0000	44	c		2.030	
S6,9-Bis(propanoyl-oxymethyl)-6-mercaptopurine	76.5	-1.440	1.900	2.50	0.00	1.64	2.2626	6.2500	0.0000	52	c		0.883	
Salicylamide	142.0	-0.796	1.160	1.65	0.63	0.48	1.0315	2.7225	0.3024	117	d	-1.754	1.129	-0.625
Salicylic acid	159.0	0.150	0.900	0.85	0.73	0.37	0.9904	0.7225	0.2701	134	b,c	-1.733	2.129	0.396
Simvastatin	136.0	-0.596	1.350	2.55	0.32	1.86	3.4268	6.5025	0.5952	111	b	-4.150	4.541	0.391
Sulfacetamide	182.0	-2.030	1.480	2.73	0.42	1.30	1.4944	7.4529	0.5460	157	r	-1.412	-1.363	-2.775
Sulfadiazine	259.0	-4.056	2.080	2.15	0.47	1.57	1.7225	4.6225	0.7379	234	c	-3.570	-0.645	-4.215
Sulfadimethoxine	204.5	-2.890	2.140	2.39	0.51	1.53	2.1217	5.7121	0.7803	180	c	-2.960	0.987	-1.973
Sulfamerazine	235.0	-3.356	2.110	2.60	0.41	1.58	1.8634	6.7600	0.6478	210	r	-3.096	-0.548	-3.644
Sulfamethazine	196.0	-2.796	2.130	2.45	0.59	1.54	2.0043	6.0025	0.9086	171	r	-2.796	0.382	-2.414
Sulfamethoxazole	168.0	-2.215	1.890	2.23	0.58	1.29	1.7244	4.9729	0.7482	143	r	-2.833	0.372	-2.461
Sulfamethoxypyridazine	182.5	-2.710	2.120	2.95	0.48	1.56	1.9221	8.7025	0.7488	158	c	-3.300	-0.576	-3.876
Sulfanilamide	166.2	-2.490	1.500	1.82	0.41	1.19	1.1969	3.3124	0.4879	141	r	-1.370	-1.192	-2.562
Sulfapyridine	190.0	-3.300	2.080	2.38	0.67	1.42	1.7636	5.6644	0.9514	165	r	-2.979	-0.076	-3.055
Sulfathiazole	200.0	-3.220	2.110	2.50	0.68	1.40	1.6883	6.2500	0.9520	175	r	-2.744	-0.420	-3.164
Sulfisomidine	243.0	-3.060	2.130	2.70	0.48	1.76	2.0043	7.2900	0.8448	218	c	-2.200	-0.811	-3.011
Sulfisoxazole	194.0	-2.450	1.900	2.26	0.65	1.35	1.8653	5.1076	0.8775	169	c	-2.900	0.686	-2.214
Sulindac	183.5	-1.730	2.260	2.75	0.61	1.41	2.5711	7.5625	0.8601	159	c	-5.000	3.074	-1.926
Sulindac ethyl ester	128.0	-1.720	2.170	2.67	0.00	1.54	2.8529	7.1289	0.0000	103	c		3.751	
Terbutryn	105.0	-0.270	1.430	1.23	0.12	0.99	1.9425	1.5129	0.1188	80	b,c	-3.711	3.382	-0.329
Testosterone	154.0	-0.474	1.540	2.56	0.32	1.17	2.3827	6.5536	0.3744	129	k	-3.972	3.142	-0.830
Testosterone benzoate	195.0	-1.320	2.050	2.30	0.00	1.31	3.1471	5.2900	0.0000	170	b,c		6.294	
Testosterone phenylacetate	129.0	-0.970	2.020	2.65	0.00	1.45	3.2880	7.0225	0.0000	104	b,c		5.915	
Testosterone phenylbutanoate	78.0	-0.050	2.020	2.76	0.00	1.48	3.5698	7.6176	0.0000	53	b,c		6.862	
Testosterone phenylpropanoate	116.5	-0.480	2.020	2.69	0.00	1.46	3.4289	7.2361	0.0000	92	b,c		6.425	
Thalidomide	275.0	-3.570	1.920	2.81	0.36	1.19	1.7479	7.8961	0.4284	250	b,c	-3.700	0.304	-3.396
Theophylline	274.0	-1.990	1.500	1.60	0.54	1.34	1.2223	2.5600	0.7236	249	b,c	-1.347	-1.490	-2.837
Thianthrene	159.0	-1.460	2.240	1.39	0.00	0.36	1.5426	1.9321	0.0000	134	d	-5.950	4.592	-1.358

Thiazafluron	136.5	-0.600	0.850	1.55	0.40	1.04	1.3909	2.4025	0.4160	112	b,c	-2.100	0.226	-1.874
Thioxanthen-9-one	211.0	0.018	1.940	1.43	0.00	0.56	1.5357	2.0449	0.0000	186	d	-5.540	3.540	-2.000
Toluene	25.0	0.674	0.601	0.52	0.00	0.14	0.8573	0.2704	0.0000	0	b	-2.250	2.740	0.490
trans-Chlordane	106.0	-0.550	2.100	1.46	0.00	0.45	2.1280	2.1316	0.0000	81	c		6.539	
trans-Stilbene	125.0	-1.100	1.450	1.04	0.00	0.34	1.5630	1.0816	0.0000	100	g	-5.800	4.742	-1.058
Triamterene	306.0	-3.674	2.950	1.56	0.82	1.70	1.8282	2.4336	1.3940	281	b		0.292	
Triazolam	234.0	-2.050	2.640	2.05	0.00	1.65	2.3265	4.2025	0.0000	209	c	-4.090	1.942	-2.148
Triphenylene	197.0	-1.770	3.000	1.71	0.00	0.42	1.8234	2.9241	0.0000	172	b,c	-6.602	5.560	-1.042
Xanthene	101.0	-0.619	1.502	1.07	0.00	0.23	1.4152	1.1449	0.0000	76	d	-5.210	4.579	-0.631
Mirex (omitted)	485.0	-0.470	3.070	1.75	0.00	1.08	2.4434	3.0625	0.0000	460	a	-6.763	5.373	-1.390

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