Estimation of the Aqueous Solubility I: Application to Organic Nonelectrolytes

NEERA JAIN, SAMUEL H. YALKOWSKY

Department of Pharmaceutical Sciences, College of Pharmacy, The University of Arizona, 1703 E. Mabel Street, Tucson, Arizona 85721

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ABSTRACT: The estimation of aqueous solubilities of organic nonelectrolytes by the General Solubility Equation (GSE) as proposed by Valvani and Yalkowsky (1980) is used in this study. The data and assumptions on which the GSE are based are reevaluated, and the equation is revised. The revised GSE is validated on a set of 580 pharmaceutically, environmentally, and industrially relevant nonelectrolytes. The revised equation has a stronger theoretical background and provides a more accurate estimation of aqueous solubility. © 2001 Wiley-Liss, Inc. and the American Pharmaceutical Association J Pharm Sci 90:234–252, 2001

Keywords: solubility; estimation; nonelectrolytes; partitioning

INTRODUCTION

Of the many methods of estimating aqueous solubility reported,[1–8] the relationship of Valvani and Yalkowsky[1] that is known as the general solubility equation (GSE) has been used most extensively in pharmacy. The wide acceptability of this relationship can be attributed to its being user friendly and relatively accurate. It requires only two inputs: the melting point (mp), which is easily measured; and the octanol–water partition coefficient (K_{ow}). The latter can be either experimentally measured or accurately calculated using software programs such as CLOGP®.[9] Methods for estimating the mp are also reported in the literature.[10–12] However, because the mp is the most frequently measured of all the physical properties, its estimation is often not necessary. Using only these two variables, a quick calculation can be made for the molar solubility of any organic nonelectrolyte.

In this study, 580 organic molecules that are not ionizable in the pH range 2–13 were used to test the original and revised versions of the GSE. A systematic deviation in the predicted values led to a reevaluation of the assumptions made in the original equation. Modifying one of the assumptions derives a revised equation. The complete derivation of the revised GSE is given in the Background Section.

Extension of the revised equation to weak electrolytes in unbuffered and buffered aqueous saturated solutions is currently under investigation, and a detailed report is in preparation.

BACKGROUND

The solubility of a solid solute in water is dependent on two factors: the crystallinity of the solute and the ability of the solute to interact with water. The inhibitory effect of crystallinity on dissolution and solubility is equal to the ratio of the solubility of the crystal to that of the liquid. The ratio is frequently called the "crystal/liquid solubility ratio", the "fugacity ratio", or simply the ideal solubility (X^{ideal}). The solubility of the liquid in water (S_w^{liquid}) must be multiplied by the ideal

Correspondence to: N. Jain (Telephone 520-626-4309; Fax: 520-626-4063; E-mail: jain@pharmacy.arizona.edu)

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solubility to get the solubility of the crystal in water (S_w^c); that is,

$$S_w^c = S_w^{liquid} \frac{X^{crystal}}{X^{liquid}} \quad (1)$$

Because the two terms on the right-hand side of eq. 1 are independent on one another, they will be discussed separately.

Ideal Solubility of a Crystalline Drug[13]

When a crystalline solute is in equilibrium with an ideal solution, the partial molar free energy of the solute, G_u^C, is equal to that in solution, G_u^{Soln}:

$$G_u^C = G_u^{Soln} \quad (2)$$

Assuming that the solution is a mixture of a hypothetical supercooled liquid solute, u, and a solvent, v, then:

$$G_u^{Soln} = G_u^{SCL} + RT \ln X_u^{ideal} \quad (3)$$

where G_u^{SCL} is the partial molar free energy of the supercooled liquid solute and X_u^{ideal} is the mole fractional solubility of the solute in an ideal solution (i.e., in a solvent of similar polarity). The free energy of the crystal is equal to that of its solutions at equilibrium saturation, so eq. 1 can be written as:

$$G_u^C = G_u^{SCL} + RT \ln X_u^{ideal} \quad (4)$$

On rearrangement, we get:

$$R \ln X_u^{ideal} = \frac{G_u^C}{T} - \frac{G_u^{SCL}}{T} = \frac{\Delta G_m}{T} \quad (5)$$

where ΔG_m is the change in free energy on melting. Differentiating with respect to X_u and applying the Gibbs–Helmholz equation gives:

$$\frac{\partial R \ln X_u^{ideal}}{\partial X_u} = \frac{\Delta H_m^{(at\,T)}}{T^2} \quad (6)$$

where ΔH_m is the heat of melting. Because the supercooled liquid is identical to the true liquid at the mp, it has an ideal mole fractional solubility of unity. Therefore, the crystal–liquid solubility ratio is equivalent to the ideal crystal mole fractional solubility. Assuming the heat of melting is independent of the temperature, integration of eq. 6 results in:

$$R \ln X_u^{ideal} = R \ln \frac{X_u^C}{X_u^{SCL}} = R \ln \frac{X_u^C}{X_u^L} = \int_{T_m}^{T} \frac{-\Delta H_m^{(at\,T)}}{T^2}\, dT \quad (7)$$

If the heat of melting is not constant, Kirchoff's law must be used. According to Kirchoffs law, the energy of an irreversible process is equal to the energy of a series of reversible processes between the same endpoints. Therefore, the irreversible enthalpy of melting at temperature, T, can be described as the sum of the enthalpies of the following three reversible processes: heating of the solid to its melting point, T_m; melting the solid at its mp; and finally cooling the liquid back to temperature, T. The heat of melting at temperature T can be related to its value at melting point, ΔH_m, by:

$$\Delta H_m^{(at\,T)} = \Delta H_m^{(at\,T_m)} + C_p^L(T_m - T) - C_p^C(T_m - T) \quad (8)$$

where C_p^L and C_p^C are the heat capacities of the liquid and the solid, respectively. Substituting eq. 8 into eq. 6 gives:

$$R \ln X_u^{ideal} = -\Delta H_m \frac{(T_m - T)}{T_{mT}} - C_p^C \frac{(T_m - T)}{T} + C_p^C \ln \frac{T_m}{T} + C_p^L \frac{(T_m - T)}{T} - C_p^L \ln \frac{T_m}{T} \quad (9)$$

which simplifies to the van't Hoff equation:

$$R \ln X_u^{ideal} = -\Delta H_m \frac{(T_m - T)}{T_m T} + \Delta Cp_m \frac{(T_m - T)}{T} - \Delta Cp_m \ln \frac{T_m}{T} \quad (10)$$

where ΔCp_m is the heat capacity difference between the solid and the liquid forms of the solute; that is, the temperature dependence of the heat of melting. Using the Gibbs relationship at the phase transition, $\Delta H_m/T_m$ can be substituted by ΔS_m, the entropy of melting. This gives:

$$R \ln X_u^{ideal} = -\Delta S_m \frac{(T_m - T)}{T} + \Delta Cp_m \left[\frac{T_m - T}{T} - \ln \frac{T_m}{T}\right] \quad (11)$$

Based on the assumption[14] that either ΔCp_m and/or the difference between the terms in the bracket are nearly zero for most compounds, eq.11 can be reduced to:

$$R \ln X_u^{ideal} = -\Delta S_m \frac{(T_m - T)}{T} \quad (12)$$

(Note that eq.12 can be obtained directly from eqs. 7 and 8 if the heat capacity term is ignored.) Converting to base 10 logarithms,

$$\log X_u^{ideal} = -\Delta S_m \frac{(T_m - T)}{2.303RT} \quad (13)$$

which at 298 K becomes:

$$\log X_u^{ideal} = \frac{-\Delta S_m (T_m - 298)}{5705.85} \quad (14)$$

Assuming that $\Delta S_m = 56.5$, as per Walden's rule, eq. 14 can be simplified to:

$$\log X_u^{ideal} = -0.01(T_m - 298) = -0.01\,(mp - 25) \quad (15)$$

where mp is the melting point in degrees Celsius. Equation 15, which expresses the ideal solubility (or the solid/liquid solubility ratio), is a simple function of mp. Note that the ideal solubility is independent of the solvent and that the term (mp – 25) is set equal to zero for liquid solutes that melt below 25°C (i.e., liquids).

Solubility and Partition Coefficient of Liquid Solutes

The ideal solubility can be used to estimate the solubility of a solute in a solvent of similar polarity (e.g., anthracene in hexyne, polyethylene glycol in ether, or glycerine in methanol). However, it does not account for differences in polarities of the solute and solvent. To accomplish this an additional term must be used.

The logarithm of the octanol–water partition coefficient will be used to account for the difference between the polarity of the solute and water. The molar octanol–water partition coefficient is defined as:

$$K_{ow} = \frac{C_o}{C_w} \quad (16)$$

and can be approximated by:

$$K_{ow} = \frac{S_o}{S_w} \quad (17)$$

or

$$\log S_w = \log S_o - \log K_{ow} \quad (18)$$

where $\log K_{ow}$ can be calculated by CLOGP®[9] or other software programs. However, calculation of $\log S_o$ requires further consideration.

Solubility in Octanol

The mole fractional solubility of a liquid solute in octanol can be calculated from regular solution theory by the Scatchard–Hildebrand equation:[15]

$$\log X_u^{liquid} = \frac{2V_u(\delta_u - \delta_{oct})\phi_{oct}^2}{2.3RT} \quad (19)$$

where V_u is the molar volume of the solute, the δ values are the solubility parameters of the solute and solvent octanol, and ϕ_{oct} is the volume fraction of octanol in the solution. However, because the solubility parameters of solutes are not generally known, this approach is not convenient. Fortunately, many solutes of pharmaceutical and environmental interest have solubility parameters close to that of octanol and thus they would be expected to form an ideal or nearly ideal solution with it. Therefore, they would by completely miscible with octanol if they were liquid.

By assuming that complete miscibility corresponds to a mole fraction of 0.5 for each component, Hildebrand[15] showed that the critical solution temperature of a regular solution of similarly sized components is given by:

$$T_c = \frac{V(\delta_c - \delta_u)^2}{2R} \quad (20)$$

where V is the average molar volume of the components. Assuming the mean volume of the solute and solvent is similar to that of octanol, the eq. 20 becomes:

$$T_c = \frac{138(\delta_u - 21.1)^2}{2R} \quad (21)$$

Complete miscibility will be obtained when the temperature is above the critical solution temperature, which will occur at room temperature if the critical temperature is <298 K. Therefore, complete miscibility will be attained if $(\delta_u - 21.1)^2 < 36$, which corresponds to $15.1 < \delta_u < 27.1$. The original version of the GSE utilized this relationship to show that any solute that has a solubility

parameter ranging from 15.1 (the value for *n*-hexane) to 27.1 (the value for methanol) would be completely miscible with octanol. This range includes the vast majority of pharmaceutically and environmentally relevant compounds.

Because the molecular weight and density of octanol are 138 and 0.827, respectively, the molarity of pure octanol is 6.3. Therefore, the molar solubility S_o of the solute in octanol is equal to:

$$S_o^{\text{liquid}} = \frac{6.3}{2} = 3.15 \quad (22)$$

and

$$\log S_o^{\text{liquid}} = 0.5 \quad (23)$$

which is similar to the relationship first observed by Hansch.[16]

The octanol solubility of a crystalline solute is equal to the product of the solubility of the liquid and the crystal liquid solubility ratio; that is:

$$S_o = S_o^{\text{liquid}} \frac{X^{\text{crystal}}}{X^{\text{liquid}}} = S_o X_u^{\text{ideal}} \quad (24)$$

and therefore,

$$\log S_o = 0.5 - 0.01\,(\text{mp} - 25) \quad (25)$$

In the original derivation of the original version of the GSE[1] it was assumed that complete miscibility in octanol was expressed as $X_o^{\text{liquid}} = 1$ and $\log X_o^{\text{liquid}} = 0$. This assumption leads to an intercept of 0.80 instead of 0.50.

General Solubility Equation

Combining eqs. 18 and 23 gives the relationship between the solubility of a liquid and its polarity (as reflected by $\log K_{ow}$); that is:

$$\log S_w^{\text{liquid}} = 0.5 - \log K_{ow} \quad (26)$$

As in the case of octanol, the solubility of a solid solute in water is equal to the product of the aqueous solubility of the liquid and the crystal liquid solubility ratio; that is:

$$S_w^{\text{solid}} = S_w^{\text{liquid}} \frac{X^{\text{crystal}}}{X^{\text{liquid}}} = 0.01\,(\text{mp} - 25) \quad (27)$$

Inserting eq. 26 into eq. 27 gives the GSE for crystalline solutes. Note that eq. 28 reduces to eq. 27 for solutes that are liquid at room temperature.

$$\log S_w^{\text{solid}} = 0.5 - 0.01\,(\text{mp} - 25) - \log K_{ow} \quad (28)$$

METHODS

The majority of the mps and intrinsic aqueous solubilities for 580 compounds was collected from the AQUASOL database[17] and a few were obtained from other sources.[18–23] The measured[9,24–27] and calculated octanol–water partition coefficients were obtained with CLOGP®[9] software.

The aqueous solubilities were calculated using both the original GSE and the revised GSE and compared with the literature values. Also, multiple linear regression analysis was performed in SAS® using the same input variables.

RESULTS AND DISCUSSION

Partition Coefficient

Partition coefficients calculated with CLOGP® were used in all solubility calculations because they are readily determined and are available for compounds that have no measured values. Figure 1 shows that the CLOGP® calculated values of 410 compounds used in this study are in good agreement with the experimental values, with an average absolute error of 0.24 log units. It should be noted that if a reliable experimental octanol–water partition coefficient is available, that value should be used rather than the one determined with CLOGP®.

Solubility and Partition Coefficient

The experimentally determined solubilities of the 322 liquids (filled circles) and 258 solids (open circles) are plotted against their octanol–water partition coefficients in Figure 2. It is clear that there is a linear relationship between the solubilities and partition coefficients of the liquids. It is also clear that most of the solids are considerably less soluble than liquids with similar partition coefficients. This relationship is especially true for the higher melting solids. When the solubilities are corrected for crystallinity (by subtracting $[-0.01(\text{mp} - 25)]$ for each solid compound), all of the data fall on a single line.

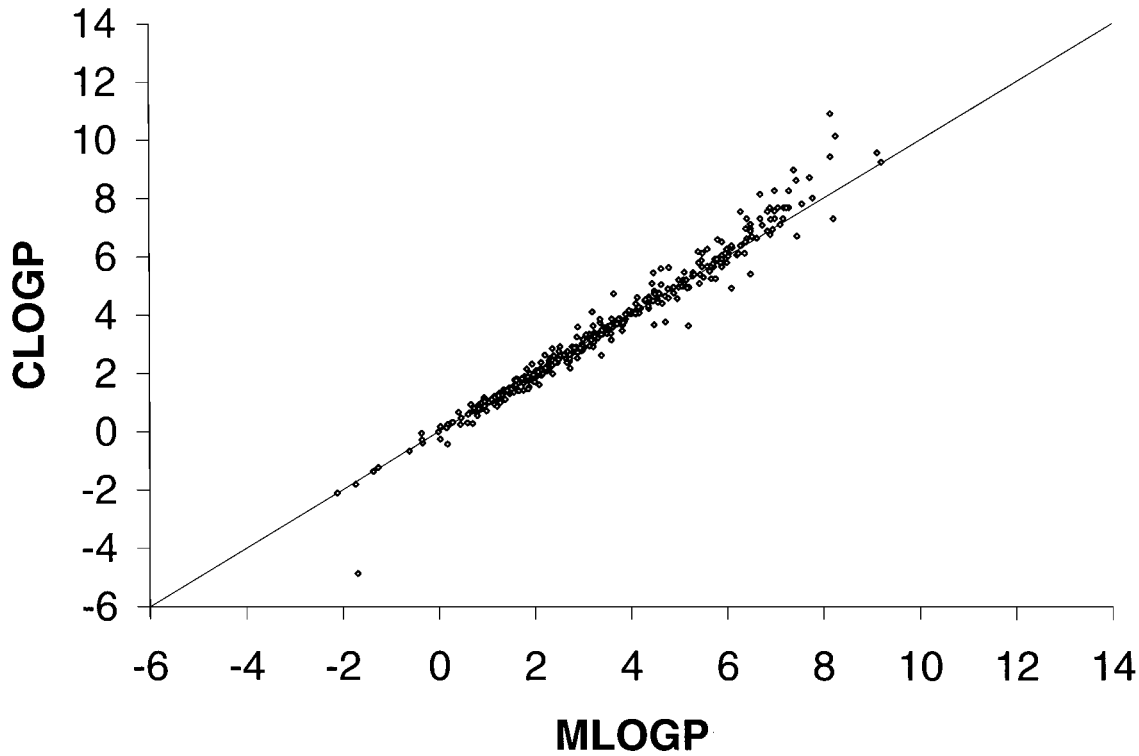

Figure 1. Measured log P versus CLOGP® ($n = 408$).

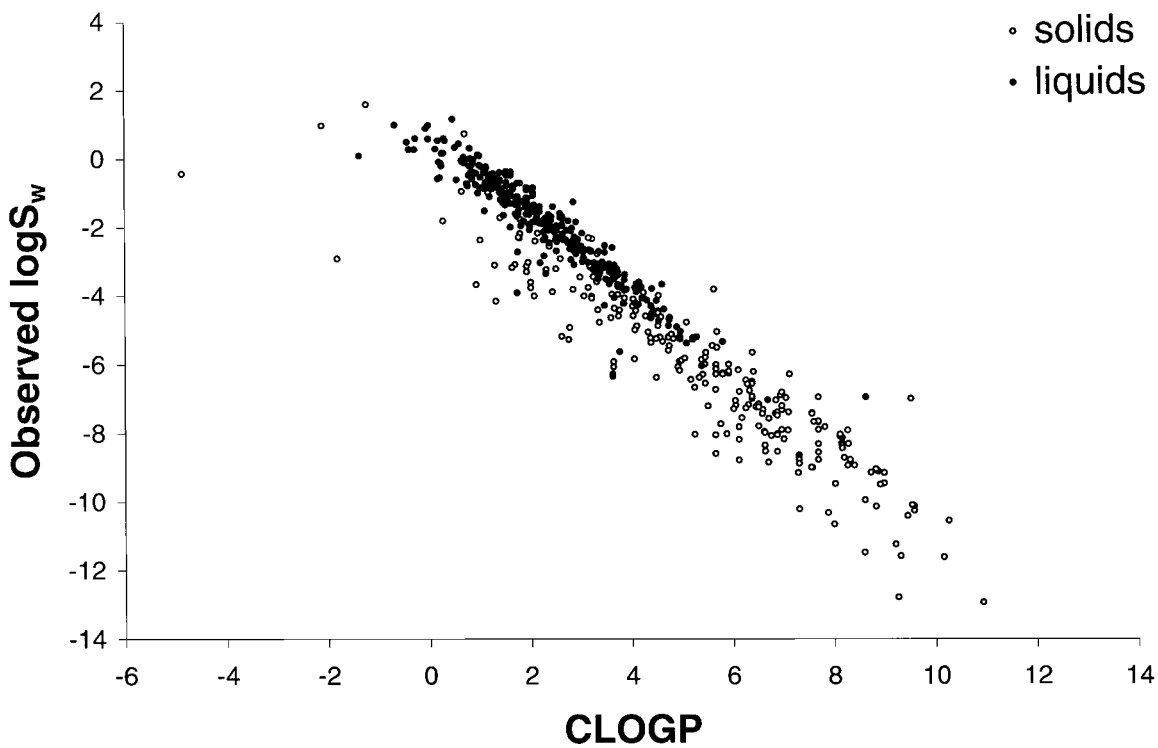

Figure 2. Experimental solubilities versus CLOGP (solids = 258, liquids = 322).

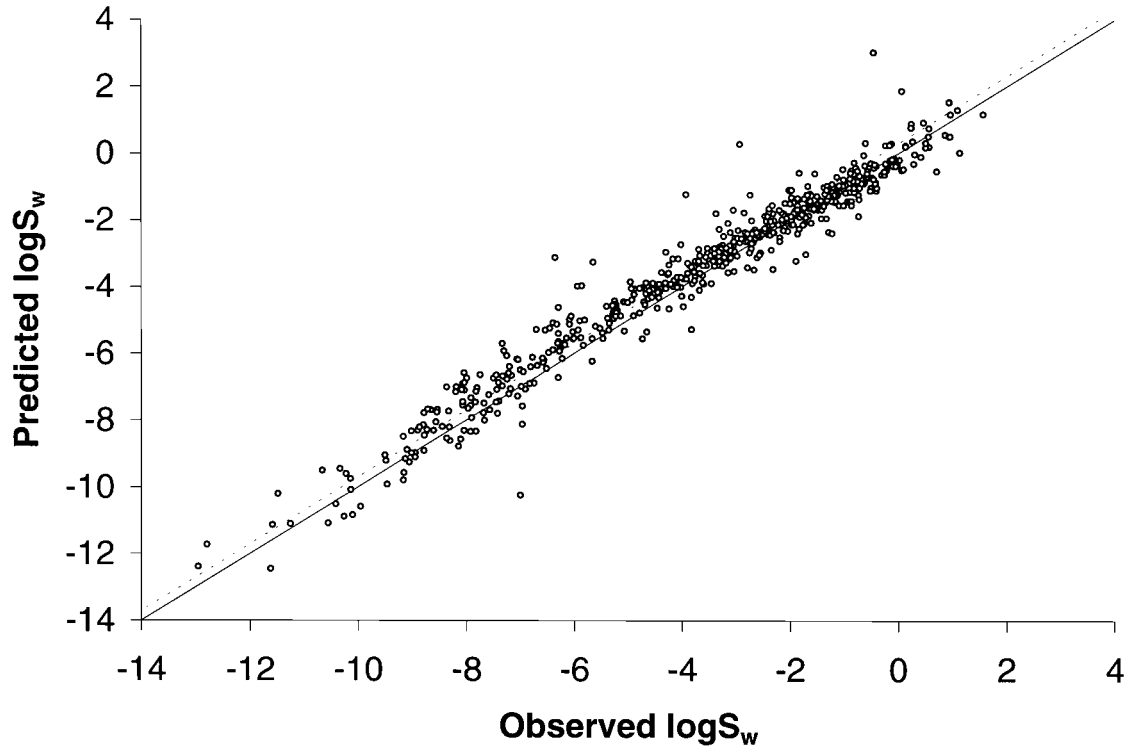

Figure 3. Experimental aqueous solubility versus calculated solubility using the original and revised GSE ($n = 580$).

Original and Revised General Solubility Equations for Nonelectrolytes

The observed and predicted aqueous solubilities of the compounds using the original and revised GSEs are listed in the Appendix. The estimated solubilities using the revised GSE versus the experimental values are plotted in Figure 3. Note that use of the originally derived equation to estimate the solubilities for the same data set gives a average absolute error (AAE) of 0.69 log units and the revised equation gives an AAE of only 0.42 log units. Thus, the revised GSE gives predictions that are ~46% more accurate than the original version (or nearly a factor of two).

The calculated solubilities for five compounds out of the 580 were >4 standard deviations (SDs) from the line. A closer look revealed that all five (cholesterol, endrin, pentaerythritol, octafluorocyclobutane, and phthalamide) had CLOGP® values that are believed to be unreliable. If the experimental values were used, the differences between the observed and experimental solubilities are 1.65 and 0.06 instead of 3.22 and 3.46 for endrin and pentaerythritol, respectively. These compounds are included in the Figure and in the Appendix, but they were not used in the calculation of the AAE. If they are included, the AAE becomes 0.44 log units. Also, the AAE is 0.47 log units when only experimental partition coefficients (MLOGP) are used instead of CLOGP® for all 410 compounds.

It is evident that the calculations using the revised GSE correspond more closely to the experimental data, which range over 16 orders of magnitude. The AAE for the total data set is only 0.42 log units. The success of the revised GSE (eq. 28) is particularly significant because it was derived without the aid of any regression-generated parameters.

Assumptions Used in the Derivation

The general solubility equation for nonelectrolytes is derived on the basis of the following assumptions:

1. The crystallinity of the solute is not affected by the presence of the solvent.
2. The entropy of melting of organic nonelectrolytes is given by Walden's rule (i.e.,

$$\Delta S_m = 56.6\,\text{J/deg mole}$$

3. The solid – liquid heat capacity[14] difference is negligible, (i.e., $\Delta Cp_m = 0$). (It should be noted that some workers prefer to assume that $\Delta Cp_m = \Delta S_m$ rather than $\Delta Cp_m = 0$. This preference leads to

$$\log X_u^{ideal} = -\frac{\Delta S_m}{2.303RT} \ln \frac{T_m}{T} \qquad (29)$$

instead of eq.13. However, because $(T_m - T)/T \approx \Delta Cp_m = 0$ for most organic nonelectrolytes, both eqs. 13 and 29 give similar results.)
4. The octanol–water partition coefficient of the solute is equal to the ratio of its solubilities in octanol and water.
5. The solute is completely miscible with octanol, and that complete miscibility is expressed as $X_o = 0.5$.

Fortunately, all the assumptions stated are valid for the vast majority of pharmaceutically, environmentally, and industrially important compounds.

Regression Analysis

It is interesting to note that regression analysis using (mp – 25) and ($\log K_{ow}$) as input parameters gives:

$$\log S_w = -0.0102\,(mp - 25 - 1.031 \log K_{ow} + 0.424$$
$$r^2 = 0.9681,\ AAE = 0.41 \qquad (30)$$

Inclusion of the five outliers would raise the AAE to 0.43.

The fact that the coefficients of (mp – 25) and $\log K_{ow}$ are extremely close to the derived values (– 0.01 and – 1.0, respectively) of the general solubility equation lends support to its validity. Boethling et al.[5] performed regression analysis using the same input parameters on an independent data set consisting of 1450 compounds and found eq. 31, which is very remarkably similar to both the theoretical and the regression equations:

$$\log S_w = -0.0107(T_m - T - 1.045 \log K_{ow} + 0.475 \qquad (31)$$

The slight difference between the constant in eq. 28 and in the intercept of eq. 30 corresponds to a factor of two and is well within the range of the experimental errors associated with the calculation of K_{ow} and the measurement of S_w.

CONCLUSIONS

A rigorous derivation of the GSE is provided that predicts double the solubility predicted by the original equation. The revised GSE is derived by defining complete miscibility as $X_o = 0.50$. It provides a better estimation of aqueous solubility (AAE of 0.44 log units) than the original GSE. Multiple regression analysis on a data set containing 580 compounds further validates the use of the revised GSE form. The Appendix is provided as supporting information.

APPENDIX

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
Acenaphthalene	363		3.62	– 3.96	– 3.47	– 3.77	0.19
Acetamide	354	– 1.26	– 1.23	1.58	1.47	1.17	– 0.41
Acetonitrile	298	– 0.34	– 0.39	0.26	1.19	0.89	0.63
Acetophenone	298	1.58	1.58	– 1.28	– 0.78	– 1.08	0.20
Acrolein	185	– 0.01	– 0.01	0.97	0.81	0.51	– 0.46
Acryladehyde	298	– 0.01	– 0.01	0.57	0.81	0.51	– 0.06
Acrylamide	189	– 0.61	– 0.67	0.98	1.47	1.17	0.19
Acrylonitrile	298	0.25	0.29	0.15	0.51	0.21	0.06
Alachlor	313	3.25	3.19	– 3.17	– 2.54	– 2.84	0.33
Aldicarb	373	1.13	1.12	– 0.71	– 1.07	– 1.37	– 0.66
Aldrin	377	6.50	5.41	– 6.30	– 5.40	– 5.70	0.60
Amylacetate	298	2.29	2.30	– 1.89	– 1.50	– 1.80	0.09

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
t-Amylbenzene	298		4.50	−4.15	−3.70	−4.00	−0.15
Androstanedione	415	3.60	3.15	−3.76	−3.52	−3.82	−0.06
Anisole	310	2.11	2.06	−1.85	−1.38	−1.68	0.17
Anthracene	489	4.45	4.49	−6.39	−5.60	−5.90	0.49
Anthraquinone	557	3.39	2.62	−5.19	−4.41	−4.71	0.48
Benzaldehyde	298	1.47	1.50	−1.19	−0.70	−1.00	0.19
Benzamide	401	0.64	0.65	−0.96	−0.88	−1.18	−0.22
Benzene	279	2.13	2.14	−1.64	−1.34	−1.64	0.00
Benzo(*a*)fluorene	460	5.68	5.25	−6.68	−6.07	−6.37	0.31
Benzo(*a*)pyrene	451	6.04	6.12	−7.82	−6.85	−7.15	0.67
Benzo(*a*)pyrene	452	5.97	6.12	−8.19	−6.86	−7.16	1.03
Benzo(*B*)fluorene	482	5.77	5.25	−8.04	−6.29	−6.59	1.45
Benzonitrile	298	1.56	1.57	−1.00	−0.77	−1.07	−0.07
Benzophenone	322	3.18	3.18	−3.12	−2.62	−2.92	0.21
Benzyl butyl phthalate	298		3.77	−5.64	−2.97	−3.27	2.37
Betamethasone	503	2.01	2.01	−3.77	−3.26	−3.56	0.21
Bibenzyl	325	4.79	4.59	−4.62	−4.06	−4.36	0.26
Bifenox	358	4.48	5.45	−6.00	−5.25	−5.55	0.45
Biphenyl	344	3.90	4.03	−4.31	−3.69	−3.99	0.32
1-Bromo-2-methylpropane	298		2.53	−2.43	−1.73	−2.03	0.40
1-Bromo-3-chloropropane	298		1.85	−1.85	−1.05	−1.35	0.50
1-Bromo-3-methylbutane	298		3.06	−2.89	−2.26	−2.56	0.33
3-Bromo-4-hydroxybenzaldehyde	397	1.83	2.15	−2.18	−2.34	−2.64	−0.46
Bromobenzene	242	2.99	3.01	−2.55	−2.21	−2.51	0.04
1-Bromobutane	298	2.75	2.66	−2.37	−1.86	−2.16	0.21
2-Bromochlorobenzene	261		3.44	−3.19	−2.64	−2.94	0.25
3-Bromochlorobenzene	252		3.72	−3.21	−2.92	−3.22	−0.01
Bromochloromethane	298	1.41	1.39	−0.89	−0.59	−0.89	0.00
Bromodichloromethane	298		2.09	−1.54	−1.29	−1.59	−0.05
Bromoethane	298	1.61	1.60	−1.09	−0.80	−1.10	−0.01
1-Bromopropane	298	2.10	2.13	−1.73	−1.33	−1.63	0.10
2-Bromopropane	298	2.14	2.13	−1.59	−1.33	−1.63	−0.04
m-Bromotoluene	233		3.50	−3.52	−2.70	−3.00	0.52
Butane	298	2.89	2.81	−2.95	−2.01	−2.31	0.64
1-Butanol	298	0.88	0.82	0.00	−0.02	−0.32	−0.32
2-Butanol	298	0.61	0.60	0.43	0.20	−0.10	−0.53
2-Butoxyethanol	298	0.82	0.83	−0.42	−0.03	−0.33	0.09
Butyl acetate	298	1.78	1.77	−1.24	−0.97	−1.27	−0.03
Butyl benzene	298	4.38	4.23	−4.06	−3.43	−3.73	0.33
t-Butyl benzene	298		4.10	−3.66	−3.30	−3.60	0.06
2-Butyl benzene	298		4.10	−3.89	−3.30	−3.60	0.29
Butyraldehyde	298	0.88	0.83	−0.01	−0.03	−0.33	−0.32
Camphor	453		2.18	−1.88	−2.93	−3.23	−1.35
Caproaldehyde	298	1.78	1.89	−1.30	−1.09	−1.39	−0.09
Caprylaldehyde	298		2.95	−2.36	−2.15	−2.45	−0.09
Carbaril	415	2.36	2.38	−2.56	−2.75	−3.05	−0.49
Carbofuran	425	1.63	1.63	−1.21	−2.10	−2.40	−1.19
Carbon tetrachloride	298	2.83	2.88	−2.29	−2.08	−2.38	−0.09
Carbophenothion	298	5.33	5.39	−6.05	−4.59	−4.89	1.16
Carboxin	365	2.14	1.93	−3.14	−1.80	−2.10	1.04
Chlordane	298	6.00	5.80	−5.35	−5.00	−5.30	0.05
Chlordene	211	5.44	5.09	−5.39	−4.29	−4.59	0.80
1-Chloro-2-bromoethane	298		1.60	−1.32	−0.80	−1.10	0.22

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
2-Chloro-2-methylbutane	298	2.52	2.92	−2.51	−2.12	−2.42	0.09
1-Chloro-2-methylpropane	298		2.39	−2.00	−1.59	−1.89	0.11
1-Chloro-4-nitrobenzene	356	2.39	2.60	−2.92	−2.38	−2.68	0.24
2-Chloroanisole	298	2.68	2.75	−2.46	−1.95	−2.25	0.21
3-Chloroanisole	298	2.98	2.91	−2.78	−2.11	−2.41	0.37
4-Chloroanisole	298	2.78	2.91	−2.78	−2.11	−2.41	0.37
Chlorobenzene	228	3.02	2.86	−2.41	−2.06	−2.36	0.05
o-Chlorobiphenyl	307	4.30	4.49	−4.54	−3.78	−4.08	0.46
m-Chlorobiphenyl	290	4.60	4.74	−4.88	−3.94	−4.24	0.64
p-Chlorobiphenyl	348	4.50	4.74	−5.20	−4.44	−4.74	0.46
1-Chlorobutane	298	2.64	2.52	−2.03	−1.72	−2.02	0.01
2-Chlorobutane	298	2.33	2.52	−1.96	−1.72	−2.02	−0.06
2-Chlorodibenzo-*p*-dioxin	362	5.45	5.39	−5.87	−5.23	−5.53	0.34
Chlorodibromomethane	298		2.23	−1.90	−1.43	−1.73	0.17
2-Chlorodiphenylether	318		5.09	−4.78	−4.49	−4.79	−0.01
1-Chlorohexane	298		3.58	−3.12	−2.78	−3.08	0.04
Chloroneb	407		3.34	−4.41	−3.63	−3.93	0.48
1-Chloropentane	298		3.05	−2.73	−2.25	2.55	0.18
2-Chloropentane	298		3.05	−2.63	−2.25	−2.55	0.08
3-Chloropentane	298		3.05	−2.63	−2.25	−2.55	0.08
Chloropicrin	298	2.09	1.61	−2.00	−0.81	−1.11	0.89
1-Chloropropane	298	2.04	1.99	−1.47	−1.19	−1.49	−0.02
2-Chloropropane	298	1.90	1.99	−1.41	−1.19	−1.49	−0.08
3-Chloropropylene	298		1.51	−1.36	−0.71	−1.01	0.35
Chlorothalonil	524	2.90	3.60	−4.65	−5.06	−5.36	−0.71
m-Chlorotoluene	225	3.28	3.35	−3.52	−2.55	−2.85	0.67
o-Chlorotoluene	238	3.42	3.35	−3.52	−2.55	−2.85	0.67
p-Chlorotoluene	281	3.33	3.35	−3.08	−2.55	−2.85	0.23
Chloroxuron	424	3.20	4.11	−4.89	−4.57	−4.87	0.02
Chlorpropham	311	3.51	3.37	−3.39	−2.70	−3.00	0.39
Cholesterol	421		9.52	−7.00	−9.95	−10.25	−3.25
Chrysene	528	5.73	5.66	−8.06	−7.16	−7.46	0.60
Corticosterone	454	1.94	2.32	−3.24	−3.08	−3.38	−0.14
Cortisone	495	1.47	1.30	−3.11	−2.47	−2.77	0.34
Coumarin	343	1.39	1.41	−1.73	−1.06	−1.36	0.37
t-Crotonaldehyde	298		0.52	0.32	0.28	−0.02	−0.34
1,4-Cyclohexadiene	224	2.30	2.39	−1.97	−1.59	−1.89	0.08
Cyclohexane	298	2.86	2.87	−3.10	−2.07	−2.37	0.73
Cyclohexanol	298	1.23	1.27	−0.44	−0.47	−0.77	−0.33
Cyclohexanone	298	0.81	0.86	−0.60	−0.06	−0.36	0.24
Cyclohexene	298	2.86	2.87	−2.59	−2.07	−2.37	0.22
Cyclopentane	298	3.00	2.79	−2.64	−1.99	−2.29	0.35
Cyclopentene	298		2.31	−2.10	−1.51	−1.81	0.29
DDD	383	6.22	6.06	−7.20	−6.11	−6.41	0.80
DDE	362	6.96	6.94	−6.90	−6.78	−7.08	−0.18
DDT	382	6.91	6.76	−8.08	−6.80	−7.10	0.98
Decachlorobiphenyl	577	8.27	10.16	−11.62	−12.15	−12.45	−0.83
Decachlorodiphenylether	494		10.93	−12.95	−12.09	−12.39	0.56
Deoxycorticosterone	414	2.88	3.25	−3.45	−3.61	−3.91	−0.46
Dexamethasone	535	2.01	2.01	−3.61	−3.58	−3.88	−0.27
Di(2-ethylhexyl)-phthalate	298	7.45	8.63	−6.96	−7.83	−8.13	−1.17
Dialifos	340		4.06	−5.85	−3.68	−3.98	1.87
Diallate	298		3.67	−4.06	−2.87	−3.17	0.89

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
Dibenzofuran	356	4.12	4.09	−4.44	−3.87	−4.17	0.27
Dibenzo-*p*-dioxin	396	4.38	4.62	−5.34	−4.80	−5.10	0.24
Dibenzothiophene	370	4.38	4.56	−5.21	−4.48	−4.78	0.43
1,2-Dibromo-3-chloropane	298		2.26	−2.38	−1.46	−1.76	0.62
1,2-Dibromobenzene	277	3.64	3.67	−3.50	−2.87	−3.17	0.33
1,3-Dibromobenzene	266	3.75	3.87	−3.54	−3.07	−3.37	0.17
1,4-Dibromobenzene	360	3.79	3.87	−4.07	−3.69	−3.99	0.08
4,4′-Dibromobiphenyl	437	5.72	5.76	−7.74	−6.35	−6.65	1.09
1,2-Dibromoethane	298	1.96	1.74	−1.68	−0.94	−1.24	0.44
1,2-Dibromoethylene	298		1.95	−1.32	−1.15	−1.45	−0.13
Dibromomethane	298	1.88	1.53	−1.17	−0.73	−1.03	0.14
1,3-Dibromopropane	298	2.37	1.99	−2.08	−1.19	−1.49	0.59
1,2-Dibromopropane	298		2.27	−2.15	−1.47	−1.77	0.38
Dibutylether	298	3.22	2.91	−1.85	−2.11	−2.41	−0.56
Dibutylketone	298		2.97	−2.59	−2.17	−2.47	0.12
o-dibutylphthalate	298	4.72	4.65	−4.40	−3.85	−4.15	0.25
Dicamba	388	2.21	2.63	−1.70	−2.73	−3.03	−1.33
2,3-Dichloro-2-methylbutane	298		2.91	−2.69	−2.11	−2.41	0.28
1,3-Dichloro-2-propanol	298		0.20	−0.11	0.60	0.30	0.41
2,3-Dichloroanisole	305	3.24	3.39	−3.31	−2.66	−2.96	0.35
2,6-Dichloroanisole	304	3.14	3.35	−3.10	−2.61	−2.91	0.19
1,2-Dichlorobenzene	256	3.44	3.43	−3.02	−2.63	−2.93	0.09
1,3-Dichlorobenzene	249	3.49	3.57	−3.07	−2.77	−3.07	0.00
1,4-Dichlorobenzene	327	3.44	3.57	−3.31	−3.06	−3.36	−0.05
2,4-Dichlorobiphenyl	298	5.10	5.21	−5.25	−4.41	−4.71	0.54
4,4′-Dichlorobiphenyl	422	5.30	5.46	−6.56	−5.90	−6.20	0.36
2,2′-Dichlorobiphenyl	334	4.90	4.96	−5.27	−4.52	−4.82	0.45
2,5-Dichlorobiphenyl	298	5.16	5.21	−5.24	−4.41	−4.71	0.53
2,4′-Dichlorobiphenyl	316	5.00	5.21	−5.28	−4.59	−4.89	0.39
3,3′-Dichlorobiphenyl	302	5.30	5.46	−5.80	−4.70	−5.00	0.80
3,4-Dichlorobiphenyl	323	5.29	5.34	−6.39	−4.79	−5.09	1.30
2,6-Dichlorobiphenyl	308	5.00	4.96	−5.21	−4.26	−4.56	0.65
1,1-Dichlorobutane	298		2.84	−2.40	−2.04	−2.34	0.06
2,3-Dichlorobutane	298		2.52	−2.70	−1.72	−2.02	0.68
2,8-Dichlorodibenzofuran	457	5.65	5.51	−7.21	−6.30	−6.60	0.61
2,7-Dichlorodibenzo-*p*-dioxin	483	6.38	6.12	−7.83	−7.17	−7.47	0.36
2,8-Dichlorodibenzo-*p*-dioxin	424	6.12	6.31	−7.18	−6.77	−7.07	0.11
Dichlorodifluoromethane	298	2.16	2.00	−1.99	−1.20	−1.50	0.49
2,6-Dichlorodiphenylether	312		5.69	−5.06	−5.03	−5.33	−0.27
2,4′-Dichlorodiphenylether	304		5.69	−5.52	−4.95	−5.25	0.27
2,4,4′-Dichlorodiphenylether	323		6.41	−6.22	−5.86	−6.16	0.06
1,1-Dichloroethane	298	1.79	1.78	−1.29	−0.98	−1.28	0.01
1,2-Dichloroethane	298	1.47	1.46	−1.06	−0.66	−0.96	0.10
1,1-Dichloroethylene	298	2.13	2.37	−1.64	−1.57	−1.87	−0.23
1,2-Dichloroethylene	298	1.86	1.77	−1.30	−0.97	−1.27	0.03
2,2′-Dichloroethylether	298	1.29	1.20	−1.12	−0.40	−0.70	0.42
Dichloromethane	298	1.25	1.25	−0.63	−0.45	−0.75	−0.12
1,3-Dichloropropane	298	2.00	1.71	−1.62	−0.91	−1.21	0.41
1,2-Dichloropropane	298	1.99	1.99	−1.60	−1.19	−1.49	0.11
4,5-Dichloroveratrole	356		2.99	−3.46	−2.77	−3.07	0.39
Diclofopmethyl	313	4.80	5.63	−3.82	−4.98	−5.28	−1.46
Dieldrin	448	5.20	3.63	−6.29	−4.33	−4.63	1.66
1,2-Diethoxyethane	298	0.66	0.93	−0.77	−0.13	−0.43	0.34

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
1,1-Diethoxyethane	298	0.84	0.93	−0.43	−0.13	−0.43	0.00
1,4-Diethylbenzene	298		4.20	−3.75	−3.40	−3.70	0.05
Diethylether	298	0.89	0.87	−0.09	−0.07	−0.37	−0.28
Diethylphthalate	298	2.47	2.54	−2.35	−1.74	−2.04	0.31
Digitoxin	529	2.83	2.76	−5.28	−4.27	−4.57	0.71
Digoxin	533	1.26	1.32	−4.16	−2.87	−3.17	0.99
1,4-Diiodobenzene	404	4.11	4.39	−5.37	−4.65	−4.95	0.42
1,2-Diiodoethylene	346		2.51	−3.22	−2.19	−2.49	0.73
Diisobutylphthalate	298	4.11	4.39	−4.66	−3.59	3.89	0.77
Diisopropylether	298	1.52	1.49	−1.10	−0.69	−0.99	0.11
Diisopropylketone	298	1.86	1.47	−1.30	−0.67	−0.97	0.33
Dimethoate	325	0.78	0.75	−0.74	−0.22	−0.52	0.22
2,5-Dimethoxybenzaldehyde	325	1.91	1.79	−2.32	−1.26	−1.56	0.76
1,5-Dimethoxydiethylether	298	−0.36	−0.06	0.88	0.86	0.56	−0.32
Dimethoxymethane	298	0.18	−0.43	0.48	1.23	0.93	0.45
2,2-Dimethyl-1-butanol	298		1.62	−1.04	−0.82	−1.12	−0.08
3,3-Dimethyl-1-butanol	298		1.62	−0.50	−0.82	−1.12	−0.62
2,2-Dimethyl-1-pentanol	298		2.15	−1.52	−1.35	−1.65	−0.13
2,4-Dimethyl-1-pentanol	298		2.15	−1.60	−1.35	−1.65	−0.05
4,4-Dimethyl-1-pentanol	298		2.15	−1.55	−1.35	−1.65	−0.10
2,2-Dimethyl-1-pentanol	326	1.31	1.09	−0.40	−0.57	−0.87	−0.47
3,3-Dimethyl-2-butanol	298	1.47	1.40	−0.62	−0.60	−0.90	−0.28
2,3-Dimethyl-2-butanol	298		1.40	−0.41	−0.60	−0.90	−0.49
2,4-Dimethyl-2-pentanol	298		1.93	−0.92	−1.13	−1.43	−0.51
2,3-Dimethyl-2-pentanol	298		1.93	−0.89	−1.13	−1.43	−0.54
2,2-Dimethyl-3-pentanol	298		1.93	−1.15	−1.13	−1.43	−0.28
2,4-Dimethyl-3-pentanol	298		1.93	−1.22	−1.13	−1.43	−0.21
2,3-Dimethyl-3-pentanol	298		1.93	−0.85	−1.13	−1.43	−0.58
N,*N*-Dimethylacetamide	298	−0.77	−0.80	1.11	1.60	1.30	0.19
1,2-Dimethylbenzene	248	3.12	3.09	−2.80	−2.29	−2.59	0.21
1,3-Dimethylbenzene	225	3.20	3.14	−2.82	−2.34	−2.64	0.18
1,4-Dimethylbenzene	286	3.15	3.14	−2.77	−2.34	−2.64	0.13
2,2-Dimethylbutane	298		3.61	−3.55	−2.81	−3.11	0.44
2,3-Dimethylbutanol	298		1.62	−0.39	−0.82	−1.12	−0.73
1,2-Dimethylcyclohexane	298		4.39	−4.30	−3.59	−3.89	0.41
1,4-Dimethylnaphthalene	281	4.37	4.31	−4.14	−3.51	−3.81	0.33
2,4-Dimethylpentane	298		4.14	−4.26	−3.34	−3.64	0.62
Dimethylphthalate	298	1.56	1.48	−1.66	−0.68	−0.98	0.68
Dimethylterephthalate	414	2.25	2.08	−4.01	−2.44	−2.74	1.27
1,4-Dipentadiene	298	2.47	2.37	−2.09	−1.57	−1.87	0.22
Diphenylether	301	4.21	4.24	−3.91	−3.47	−3.77	0.14
Diphenylmethane	299	4.14	4.21	−4.08	−3.42	−3.72	0.36
Dipropylether	298	2.03	1.93	−1.62	−1.13	−1.43	0.19
Enanthaldehyde	298		2.42	−1.70	−1.62	−1.92	−0.22
b-Endosulfan	482	3.83	3.65	−6.08	−4.69	−4.99	1.09
a-Endosulfan	382	3.83	3.65	−5.93	−3.69	−3.99	1.94
Endrin	253	5.20	3.63	−6.35	−2.83	−3.13	3.22
Epichlorohydrin	216	0.45	0.24	−0.15	0.56	0.26	0.41
EPTC	298	3.21	3.21	−2.70	−2.41	−2.71	−0.01
Ethane	298	1.81	1.75	−2.73	−0.95	−1.25	1.48
4-Ethoxy-3-methoxybenzaldehyde	338	1.63	1.80	−2.19	−1.40	−1.70	0.49
3-Ethoxy-4-hydroxybenzaldehyde	351	1.61	1.80	−1.77	−1.53	−1.83	−0.06
2-Ethyl-1-butanol	298		1.75	−1.17	−0.95	−1.25	−0.08

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
2-Ethyl-1-hexanol	298		2.81	− 2.11	− 2.01	− 2.31	− 0.20
1-Ethyl-2-methylbenzene	298	3.53	3.62	− 3.21	− 2.82	− 3.12	0.09
2-Ehyl-2-propanol	298	0.89	1.00	0.08	− 0.20	− 0.50	− 0.58
3-ethyl-3-pentanol	298		2.06	− 0.85	− 1.26	− 1.56	− 0.71
1-Ethyl-4-methylbenzene	298		3.67	− 3.11	− 2.87	− 3.17	− 0.06
Ethylacetate	298	0.73	0.71	− 0.04	0.09	− 0.21	− 0.17
Ethylacrylate	298	1.32	1.33	− 0.74	− 0.53	− 0.83	− 0.09
Ethylbenzoate	298	2.64	2.64	− 2.32	− 1.84	− 2.14	0.18
Ethylbutyrate	298		1.77	− 1.28	− 0.97	− 1.27	0.01
Ethylcaprylate	298		3.88	− 3.39	− 3.08	− 3.38	0.01
Ethylenedichloride	298	1.47	1.46	− 1.08	− 0.66	− 0.96	0.12
Ethylene glycol	260	− 1.36	− 1.37	0.08	2.17	1.87	1.79
Ethyl formate	298		0.26	0.15	0.54	0.24	0.09
Ethyl heptylate	298		3.36	− 2.71	− 2.56	− 2.86	− 0.15
Ethyl isopropylether	298		1.18	− 0.55	− 0.38	− 0.68	− 0.13
Ethyl pelargonate	298		4.41	− 3.80	− 3.61	− 3.91	− 0.11
Ethyl propionate	298	1.21	1.24	− 0.66	− 0.44	− 0.74	− 0.08
Ethyl propylether	298		1.40	− 0.66	− 0.60	− 0.90	− 0.24
Ethyl valerate	298		2.30	− 1.75	− 1.50	− 1.80	− 0.05
Ethyl vinylether	298	1.04	1.01	− 0.85	− 0.21	− 0.51	0.34
Eucalyptol	298	2.50	2.76	− 1.82	− 1.96	− 2.26	− 0.44
Fenfuram	383		1.93	− 3.30	− 1.98	− 2.28	1.02
Fluoranthene	383	5.22	4.95	− 5.92	− 5.00	− 5.30	0.62
Fluorene	389	4.18	4.07	− 5.00	− 4.18	− 4.48	0.52
1-Fluoro-4-iodobenzene	300		3.41	− 3.13	− 2.63	− 2.93	0.20
Fluorodifen	363	3.65	4.74	− 5.22	− 4.59	− 4.89	0.33
Flurobenzene	231	2.28	2.27	− 1.80	− 1.47	− 1.77	0.03
Furan	298	1.34	1.32	− 0.82	− 0.52	− 0.82	0.00
Furfural	298	0.41	0.67	− 0.10	0.13	− 0.17	− 0.07
Halothane	298	2.30	2.45	− 1.41	− 1.65	− 1.95	− 0.54
Heptachlor	369	6.10	4.92	− 6.08	− 4.83	− 5.13	0.95
2,2′,3,4,4′,5′,6-Heptachlorobiphenyl	356	7.30	8.27	− 7.92	− 8.05	− 8.35	− 0.43
2,2′,3,3′,4′,4′,6-Heptachlorobiphenyl	395	6.70	8.15	− 8.30	− 8.32	− 8.62	− 0.32
2,2′,3,4′,5,5′,6-Heptachlorobiphenyl	420	7.00	8.27	− 8.94	− 8.69	− 8.99	− 0.05
1,2,3,4,6,7,8-Heptachlorodibenzofuran	509		8.60	− 11.48	− 9.91	− 10.21	1.27
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	538		9.21	− 11.25	− 10.81	− 11.11	0.14
2,3,3′,4,4′,5,6-Heptachlorodiphenylether	442		8.99	− 9.46	− 9.63	− 9.93	− 0.47
2,2′,3,3′,4,4′,5-Heptachlorodiphenylether	377		8.87	− 9.12	− 8.86	− 9.16	− 0.04
2,2′,3,4,4′,5,5′-Heptachlorodiphenylether	362		8.91	− 9.50	− 8.75	− 9.05	0.45
2,2′,3,3′,4′,5,6-Heptachlorodiphenylether	354		8.83	− 9.09	− 8.59	− 8.89	0.20
2,2′,3,4′,5,5′,6-Heptachlorodiphenylether	391		8.83	− 9.05	− 8.96	− 9.26	− 0.21
Heptane	298	4.66	4.40	− 4.53	− 3.60	− 3.90	0.63
1-Heptanol	298	2.72	2.41	− 1.81	− 1.61	− 1.91	− 0.10
2-Heptanol	298	2.31	2.19	− 1.55	− 1.39	− 1.69	− 0.14
3-Heptanol	298	2.24	2.19	− 1.47	− 1.39	− 1.69	− 0.22
4-Heptanol	298	2.22	2.19	− 1.40	− 1.39	− 1.69	− 0.29
trans-2-Heptene	298		3.91	− 3.82	− 3.11	− 3.41	0.41
1-Heptyne	298		3.04	− 3.01	− 2.24	− 2.54	0.47
Hexachloro-1,3-butadiene	298	4.78	4.90	− 4.92	− 4.10	− 4.40	0.52
Hexachlorobenzene	500	5.41	6.18	− 7.56	− 7.40	− 7.70	− 0.14
2,2′,4,4′,5,5′-Hexachlorobiphenyl	385	6.90	7.69	− 8.56	− 7.76	− 8.06	0.50
2,2′,3,3′,6,6′-Hexachlorobiphenyl	387	6.70	7.31	− 8.65	− 7.40	− 7.70	0.95
2,2′,3,3′,5,5′-Hexachlorobiphenyl	338	7.07	7.69	− 6.96	− 7.29	− 7.59	− 0.63

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
2,2′,4,4′,6,6′-Hexachlorobiphenyl	386	7.00	7.31	−8.71	−7.39	−7.69	1.03
2,2′,3,3′,4,4′-Hexachlorobiphenyl	425	7.00	7.57	−9.01	−8.04	−8.34	0.67
2,2′,3,3′,4,5-Hexachlorobiphenyl	358	7.30	7.69	−8.78	−7.49	−7.79	0.99
2,2′,3,4,4′,5′-Hexachlorobiphenyl	353	7.25	7.69	−8.32	−7.44	−7.74	0.58
2,2′,3,4,5,5′-Hexachlorobiphenyl	358	7.19	7.69	−7.68	−7.49	−7.79	−0.11
2,2′,3,5,5′,6-Hexachlorobiphenyl	373	6.85	7.56	−7.42	−7.51	−7.81	−0.39
2,3,3′,4,4′,5-Hexachlorobiphenyl	400	7.57	7.82	−7.82	−8.04	−8.34	−0.52
2,3,3′,4,4′,6-Hexachlorobiphenyl	380	7.25	7.69	−7.66	−7.71	−8.01	−0.35
2,2′,3,3′,5,6-Hexachlorobiphenyl	373	7.25	7.69	−7.90	−7.64	−7.94	−0.04
1,2,3,6,7,8-Hexachlorodibenzofuran	506		7.88	−10.33	−9.16	−9.46	0.87
1,2,3,4,7,8-Hexachlorodibenzofuran	499		8.00	−10.66	−9.21	−9.51	1.15
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	546		8.61	−9.95	−10.29	−10.59	−0.64
2,2′,3,3′,4,4′-Hexachlorodiphenylether	411		8.16	−8.14	−8.49	−8.79	−0.65
2,2′,3,4,4′,6′-Hexachlorodiphenylether	394		8.12	−8.10	−8.28	−8.58	−0.48
2,2′,3,4,4′,5′-Hexachlorodiphenylether	342		8.28	−8.31	−7.92	−8.22	0.09
2,2′,4,4′,5,5′-Hexachlorodiphenylether	387		8.16	−8.36	−8.25	−8.55	−0.19
2,2′,4,4′,5,6′-Hexachlorodiphenylether	368		8.12	−8.04	−8.02	−8.32	−0.28
2,3′,4,4′,5,5′-Hexachlorodiphenylether	357		8.20	−8.72	−7.99	−8.29	0.43
2,2′,3′,4,4′,5-Hexachlorodiphenylether	352		8.16	−8.44	−7.90	−8.20	0.24
2,3,3′,4,4′,5-Hexachlorodiphenylether	408		8.32	−8.78	−8.62	−8.92	−0.14
2,3,4,4′,5,6-Hexachlorodiphenylether	419		8.40	−8.94	−8.81	−9.11	−0.17
Hexachloroethane	298	4.14	4.61	−3.67	−3.81	−4.11	−0.44
1,5-Hexadiene	298	2.87	2.90	−2.68	−2.10	−2.40	0.28
Hexane	298	3.90	3.87	−3.84	−3.07	−3.37	0.47
1-Hexanol	298	2.03	1.88	−1.24	−1.08	−1.38	−0.14
2-Hexanol	298	1.76	1.66	−0.89	−0.86	−1.16	−0.27
3-Hexanol	298	1.65	1.66	−0.80	−0.86	−1.16	−0.36
1-Hexene	298	3.39	3.38	−3.23	−2.58	−2.88	0.35
Hexyl acetate	298	2.96	2.83	−2.46	−2.03	−2.33	0.13
Hexyl benzene	298	5.52	5.29	−5.21	−4.49	−4.79	0.42
1-Hexyne	298	2.73	2.51	−2.36	−1.71	−2.01	0.35
Hydrocortisone	491	1.61	1.70	−3.09	−2.83	−3.13	−0.04
p-Hydroxybenzaldehyde	298	1.35	1.44	−0.96	−0.64	−0.94	0.02
11-*a*-Hydroxyprogesterone	495	2.36	2.85	−3.82	−4.02	−4.32	−0.50
Indane	298	3.18	3.15	−3.03	−2.35	−2.65	0.38
Iodobenzene	244	3.25	3.27	−3.04	−2.47	−2.77	0.27
1-Iodobutane	298		3.05	−2.96	−2.25	−2.55	0.41
Iodoethane	298	2.00	2.00	−1.60	−1.20	−1.50	0.10
Iodomethane	298	1.51	1.47	−1.00	−0.67	−0.97	0.03
1-Iodopropane	298		2.52	−2.29	−1.72	−2.02	0.27
2-Iodopropane	298	2.89	2.52	−2.09	−1.72	−2.02	0.07
Isobutylacetate	298	1.76	1.42	−1.21	−0.62	−0.92	0.29
Isobutylformate	298		0.97	−1.01	−0.17	−0.47	0.54
Isopentanol	298	1.16	1.22	−0.52	−0.42	−0.72	−0.20
Isopropylacetate	298	1.22	1.02	−0.55	−0.22	−0.52	0.03
p-Isopropyltoluene	298	4.10	4.07	−3.77	−3.27	−3.57	0.20
Leptophos	333	6.31	6.39	−5.66	−5.94	−6.24	−0.58
Lindane	386	3.72	3.75	−4.43	−3.83	−4.13	0.30
Lindane	385	3.72	3.75	−4.60	−3.82	−4.12	0.48
Malathion	276	2.38	2.31	−3.36	−1.51	−1.81	1.55
Malonicaciddiethylester	298	0.96	1.13	−0.82	−0.33	−0.63	0.19
Menthol	315		3.23	−2.34	−2.60	−2.90	−0.56
Meprobamate	378	0.70	0.28	−1.82	−0.28	−0.58	1.24

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
Methane	90	1.09	1.10	−1.53	−0.30	−0.60	0.93
p-Methoxybenzaldehyde	298	1.76	1.78	−1.49	−0.98	−1.28	0.21
Methoxybenzene	298	2.11	2.06	−1.85	−1.26	−1.56	0.29
Methoxychlor	356	5.08	5.17	−6.45	−4.95	−5.25	1.20
2-Methyl-1,3-butadiene	298		2.83	−2.03	−2.03	−2.33	−0.30
2-Methyl-1-butanol	298		1.22	−0.47	−0.42	−0.72	−0.25
2-Methyl-1-pentanol	298		1.75	−1.11	−0.95	−1.25	−0.14
4-Methyl-1-pentanol	298		1.75	−1.14	−0.95	−1.25	−0.11
4-Methyl-1-pentene	298		3.25	−3.24	−2.45	−2.75	0.49
3-Methyl-2-butanol	298	1.28	1.00	−0.20	−0.20	−0.50	−0.30
3-Methyl-2-heptanol	298		2.59	−1.72	−1.79	−2.09	−0.37
2-Methyl-2-heptanol	298		2.59	−1.72	−1.79	−2.09	−0.37
5-Methyl-2-hexanol	298		2.06	−1.38	−1.26	−1.56	−0.18
2-Methyl-2-hexanol	298		2.06	−1.08	−1.26	−1.56	−0.48
4-Methyl-2-pentanol	298		1.53	−0.80	−0.73	−1.03	−0.23
2-Methyl-2-pentanol	298		1.53	−0.49	−0.73	−1.03	−0.54
3-Methyl-2-pentanol	298		1.75	−0.72	−0.95	−1.25	−0.53
3-Methyl-3-heptanol	298		2.59	−1.60	−1.79	−2.09	−0.49
3-Methyl-3-hexanol	298		2.06	−1.00	−1.26	−1.56	−0.56
2-Methyl-3-pentanol	298		1.53	−0.70	−0.73	−1.03	−0.33
3-Methyl-3-pentanol	298		1.53	−0.38	−0.73	−1.03	−0.65
Methyl acetate	298	0.18	0.18	−0.52	0.62	0.32	−0.20
Methyl acrylate	298	0.80	0.80	−0.22	0.00	−0.30	−0.08
9-Methyl anthracene	352	5.07	4.99	−5.89	−4.73	−5.03	0.86
Methyl benzoate	298	2.12	2.11	−1.85	−1.31	−1.61	0.24
Methyl bromide	179	1.19	1.08	−0.87	−0.28	−0.58	0.29
Methyl butylether	298	1.66	1.40	−0.99	−0.60	−0.90	0.09
Methyl butylketone	298	1.38	1.38	−0.80	−0.58	−0.88	−0.08
Methyl butyrate	298	1.29	1.24	−0.82	−0.44	−0.74	0.08
Methyl caprylate	298		3.36	−3.39	−2.56	−2.86	0.53
Methyl chloride	176	1.25	1.25	−0.88	−0.45	−0.75	0.13
3-Methyl cholanthrene	452	6.42	6.62	−7.96	−7.36	−7.66	0.30
Methyl cyclohexane	298	3.61	3.87	−3.85	−3.07	−3.37	0.48
Methyl cyclohexene	298		3.39	−3.27	−2.59	−2.89	0.38
Methyl cyclopentane	298	3.37	3.31	−3.30	−2.51	−2.81	0.49
Methyl ethyl ketone	298	0.29	0.32	0.52	0.48	0.18	−0.34
1-Methyl fluorene	360	4.97	4.57	−5.22	−4.39	−4.69	0.53
Methyl formate	298	0.03	−0.26	0.58	1.06	0.76	0.18
Methyl heptyl ketone	298	3.14	2.94	−2.58	−2.14	−2.44	0.14
Methyl hexyl ketone	298	2.37	2.44	−2.05	−1.64	−1.94	0.11
Methyl iodide	209	1.51	1.47	−1.01	−0.67	−0.97	0.04
Methyl isobutyl ketone	298	1.31	1.25	−0.74	−0.45	−0.75	−0.01
Methyl isopropyl ether	298		0.65	−0.06	0.15	−0.15	−0.09
Methyl isothiocyanate	309	0.94	1.17	−1.00	−0.48	−0.78	0.22
Methyl methacrylate	298	1.38	1.11	−0.80	−0.31	−0.61	0.19
1-Methyl naphthalene	251	3.87	3.81	−3.70	−3.01	−3.31	0.39
2-Methyl naphthalene	307	3.86	3.81	−3.77	−3.10	−3.40	0.37
2-Methyl pentane	298		3.74	−3.74	−2.94	−3.24	0.50
3-Methyl pentane	298		3.74	−3.68	−2.94	−3.24	0.44
Methyl pentylketone	298	1.98	1.91	−1.42	−1.11	−1.41	0.01
Methyl prednisolone	506		1.96	−3.03	−3.24	−3.54	−0.51
2-Methyl propanol	298	0.76	0.69	0.04	0.11	−0.19	−0.23
Methyl propionate	298	0.82	0.71	−0.14	0.09	−0.21	−0.07

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
Methyl propyl ether	298	1.21	0.87	−0.39	−0.07	−0.37	0.02
Methyl propyl ketone	298	0.91	0.85	−0.19	−0.05	−0.35	−0.16
Methyl-*t*-butylether	298	0.95	1.04	−0.24	−0.24	−0.54	−0.30
17-Methyl testosterone	434	3.36	3.74	−3.97	−4.30	−4.60	−0.63
2-Methyl tetrahydrofuran	298		0.97	0.11	−0.17	−0.47	−0.58
Methyl valerate	298		2.08	−1.36	−1.28	−1.58	−0.22
Myristyl Alcohol	311		6.11	−6.17	−5.44	−5.74	0.43
Naphthacene	614	5.90	5.66	−8.60	−8.02	−8.32	0.28
Naphthalene	353	3.30	3.32	−3.60	−3.07	−3.37	0.23
o-Nitroanisole	298	1.73	1.82	−1.96	−1.02	−1.32	0.64
p-Nitroanisole	327	2.03	2.10	−2.41	−1.59	−1.89	0.52
Nitrobenzene	278	1.85	1.88	−1.83	−1.08	−1.38	0.45
Nitroethane	298	0.18	0.25	−0.22	0.55	0.25	0.47
Nitrofen	344	4.64	5.60	−5.46	−5.26	−5.56	−0.09
Nitromethane	298	−0.35	−0.28	0.26	1.08	0.78	0.52
1-Nitropropane	298	0.87	0.77	−0.80	0.03	−0.27	0.53
2-Nitropropane	298	0.80	0.55	−0.62	0.25	−0.05	0.57
m-Nitrotoluene	288	2.42	2.38	−2.46	−1.58	−1.88	0.58
o-Nitrotoluene	269	2.30	2.30	−2.31	−1.50	−1.80	0.51
2,2′,3,3′,4,4′,5,5′,6′-Nonachlorobiphenyl	479	9.14	9.58	−10.26	−10.59	−10.89	−0.63
2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl	455	8.16	9.45	−10.41	−10.22	−10.52	−0.11
2,2′,3,3′,4,4′,5,5′6′-Nonachlorodiphenylether	431		10.26	−10.55	−10.79	−11.09	−0.54
1-Nonene	298	5.15	4.97	−5.05	−4.17	−4.47	0.58
1-Nonyne	298		4.10	−4.24	−3.30	−3.60	0.64
Norethindrone	476	2.97	2.78	−4.93	−3.76	−4.06	0.87
2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl	429	7.40	8.99	−9.16	−9.50	−9.80	−0.64
2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl	433	7.73	8.73	−9.15	−9.28	−9.58	−0.43
Octachlorodibenzofuran	531		9.31	−11.59	−10.84	−11.14	0.45
Octachlorodibenzo-p-dioxin	595	9.22	9.26	−12.79	−11.43	−11.73	1.06
2,2′,3,4,4′,5,5′,6-Octachlorodiphenylether	411		8.83	−10.14	−9.46	−9.76	0.38
2,2′,3,3′,4,4′,5,5′-Octachlorodiphenylether	399		9.58	−10.13	−9.79	−10.09	0.04
2,2′,3,3′,4,5,5′,6′-Octachlorodiphenylether	478		9.54	−10.10	−10.54	−10.84	−0.74
Octafluorocyclobutane	232		1.74	−3.92	−0.94	−1.24	2.68
Octane	298	5.18	4.93	−5.24	−4.13	−4.43	0.81
1-Octanol	298	3.00	2.94	−2.39	−2.14	−2.44	−0.05
2-Octanol	298	2.90	2.72	−2.09	−1.92	−2.22	−0.13
1-Octene	298	4.57	4.44	−4.44	−3.64	−3.94	0.50
1-Octyne	298		3.57	−3.66	−2.77	−3.07	0.59
Parathion	279	3.83	3.47	−4.29	−2.67	−2.97	1.32
Pebulate	298	3.84	3.74	−3.41	−2.94	−3.24	0.17
Pelargonaldehyde	298		3.48	−3.17	−2.68	−2.98	0.19
1,1,3,4,4-Pentachloro-1,2-butadi	298		3.85	−4.23	−3.05	−3.35	0.88
Pentachlorobenzene	357	5.12	5.47	−5.66	−5.26	−5.56	0.10
2,2′,4,5,5′-Pentachlorobiphenyl	350	6.40	6.97	−7.33	−6.69	−6.99	0.35
2,2′,3,4,5-Pentachlorobiphenyl	373		6.97	−7.21	−6.92	−7.22	−0.01
2,2′,3,4,5′-Pentachlorobiphenyl	385	6.50	6.97	−7.91	−7.04	−7.34	0.57
2,3,4,5,6-Pentachlorobiphenyl	397	6.74	7.09	−7.92	−7.28	−7.58	0.34
2,2′,3,4,6-Pentachlorobiphenyl	373		6.84	−7.43	−6.79	−7.09	0.34
2,2′,4,6,6′-Pentachlorobiphenyl	358	5.81	6.59	−7.32	−6.39	−6.69	0.63
2,2′,3,3′,4-Pentachlorobiphenyl	392		6.85	−7.05	−6.99	−7.29	−0.24
2,3′,4,4′,5-Pentachlorobiphenyl	382	7.12	7.10	−7.39	−7.14	−7.44	−0.05
2,3,4,7,8-Pentachlorodibenzofuran	469	6.92	7.29	−9.16	−8.20	−8.50	0.66
1,2,3,4,7-Pentachlorodibenzo-p-dioxin	468	7.79	8.02	−9.48	−8.92	−9.22	0.26

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
2,2′,3,4,4′-Pentachlorodiphenylether	339		7.56	− 7.44	− 7.17	− 7.47	− 0.03
2,3,3′,4,4′-Pentachlorodiphenylether	338		7.60	− 7.67	− 7.20	− 7.50	0.17
Pentachloroethane	298	3.22	3.63	− 2.60	− 2.83	− 3.13	− 0.53
Pentaerythritol	533		− 4.87	− 0.44	3.32	3.02	3.46
Pentamethylbenzene	323	4.56	4.54	− 4.00	− 3.99	− 4.29	− 0.29
Pentane	298	3.39	3.34	− 3.18	− 2.54	− 2.84	0.34
Mentanochlor	359	4.31	4.53	− 4.45	− 4.34	− 4.64	− 0.19
1-Mentanol	298	1.56	1.35	− 0.60	− 0.55	− 0.85	− 0.25
2-Mentanol	298	1.19	1.13	− 0.29	− 0.33	− 0.63	− 0.34
3-Mentanol	298	1.21	1.13	− 0.24	− 0.33	− 0.63	− 0.39
1-Pentene	298		2.86	− 2.68	− 2.06	− 2.36	0.32
Trans-2-pentene	298		2.86	− 2.54	− 2.06	− 2.36	0.18
Pentylbenzene	298	4.90	4.76	− 4.64	− 3.96	− 4.26	0.38
1-Pentyne	298	1.98	1.98	− 1.64	− 1.18	− 1.48	0.16
Permethrin	309	6.50	7.12	− 6.29	− 6.43	− 6.73	− 0.44
Perthane	292		6.69	− 7.04	− 5.89	− 6.19	0.85
Perylene	551	6.25	6.12	− 8.79	− 7.85	− 8.15	0.64
Phenacetin	408	1.58	1.77	− 2.30	− 2.07	− 2.37	− 0.07
Phenanthrene	372	4.47	4.49	− 5.26	− 4.43	− 4.73	0.53
Phenmedipham	416	3.59	3.37	− 4.78	− 3.75	− 4.05	0.73
2-Phenoxyethanol	298	1.16	1.17	− 0.70	− 0.37	− 0.67	0.03
Phenylbutazone	380	3.16	3.16	− 2.31	− 3.18	− 3.48	− 1.17
1-Phenylethanol	298	1.42	1.41	− 0.92	− 0.61	− 0.91	0.01
Phenylmethanol	298	1.10	1.10	− 0.40	− 0.30	− 0.60	− 0.20
Phthalamide	501	− 1.73	− 1.81	− 2.92	0.58	0.28	3.20
Phthalonitrile	413	0.99	1.01	− 2.38	− 1.36	− 1.66	0.72
Prasterone	414	3.23	3.07	− 4.01	− 3.43	− 3.73	0.28
Prednisolone	513	1.62	1.64	− 3.18	− 2.99	− 3.29	− 0.11
Progesterone	404	3.87	3.77	− 4.42	− 4.03	− 4.33	0.09
Propane	298	2.36	2.28	− 2.84	− 1.48	− 1.78	1.06
Propanil	358	3.07	3.33	− 2.78	− 3.13	− 3.43	− 0.65
Propionaldehyde	298	0.59	0.30	0.58	0.50	0.20	− 0.38
Propionitrile	298	0.16	0.13	0.28	0.67	0.37	0.09
Propyl acetate	298	1.24	1.24	− 0.72	− 0.44	− 0.74	− 0.02
Propyl benzene	298	3.72	3.70	− 3.37	− 2.90	− 3.20	0.17
Propyl benzoate	298	3.01	3.17	− 2.67	− 2.37	− 2.67	0.00
Propyl butyrate	298		2.30	− 1.92	− 1.50	− 1.80	0.12
Propylene oxide	298	0.03	0.18	− 0.59	0.62	0.32	0.91
Propyl formate	298	0.83	0.79	− 0.49	0.01	− 0.29	0.20
Propyl isopropyl ether	298		1.71	− 1.34	− 0.91	− 1.21	0.13
Propyzamide	429	3.36	3.86	− 4.23	− 4.37	− 4.67	− 0.44
Pyrene	423	5.18	4.95	− 6.18	− 5.40	− 5.70	0.48
Quinone	386	0.20	0.22	− 0.56	− 0.30	− 0.60	− 0.04
Quintozene	419	4.64	5.05	− 5.82	− 5.46	− 5.76	0.06
Styrene	243	2.95	2.87	− 2.61	− 2.07	− 2.37	0.24
Styrene oxide	298	1.61	1.76	− 1.60	− 0.96	− 1.26	0.34
TCDD	578	6.42	7.31	− 10.22	− 9.31	− 9.61	0.61
Testosterone	428	3.32	3.22	− 4.02	− 3.72	− 4.02	0.00
Testosterone	428	3.32	3.22	− 4.08	− 3.72	− 4.02	0.06
2,2′,5,5′-Tetrabromobiphenyl	416	6.50	6.88	− 8.06	− 7.26	− 7.56	0.50
1,1,2,2-Tetrabromoethane	298		3.20	− 2.72	− 2.40	− 2.70	0.02
Tetrabromomethane	363	3.42	3.43	− 3.14	− 3.28	− 3.58	− 0.44
2,4,3,5-Tetrachloroanisole	361	4.50	4.83	− 5.26	− 4.66	− 4.96	0.30

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
2,4,5,6-Tetrachloroanisole	357		4.79	−5.13	−4.58	−4.88	0.25
1,2,3,4-Tetrachlorobenzene	319	4.55	4.75	−4.70	−4.16	−4.46	0.24
1,2,3,5-Tetrachlorobenzene	327	4.59	4.75	−4.68	−4.24	−4.54	0.14
1,2,4,5-Tetrachlorobenzene	412	4.60	4.75	−5.47	−5.09	−5.39	0.08
2,2′,4,6′-Tetrachlorobenzyl-3-toluene	360		6.63	−7.99	−6.45	−6.75	1.24
2,2′,4,4′-Tetrachlorobenzyl-3-toluene	349		6.88	−7.40	−6.59	−6.89	0.51
2,2′,5,5′-Tetrachlorobenzyl-4-toluene	348		6.88	−8.03	−6.58	−6.88	1.15
2,2′,4,6′-Tetrachlorobenzyl-5-toluene	387		6.63	−8.36	−6.72	−7.02	1.34
2,2′4,5′-Tetrachlorobenzyl-5-toluene	352		6.88	−8.06	−6.62	−6.92	1.14
2,2′,4,4′-Tetrachlorobenzyl-5-toluene	335		6.88	−7.49	−6.45	−6.75	0.74
2,3,4,4′-Tetrachlorobenzyl-5-toluene	348		7.01	−8.18	−6.71	−7.01	1.17
2,3,4,6′-Tetrachlorobenzyl-6-toluene	380		6.46	−7.24	−6.48	−6.78	0.46
2,3,4,4′-Tetrachlorobenzyl-6-toluene	356		6.58	−7.44	−6.36	−6.66	0.78
2,2′,3,3′-Tetrachlorobiphenyltoluene	394	5.60	6.26	−7.28	−6.42	−6.72	0.56
2,2′,4,4′-Tetrachlorobiphenyltoluene	356	6.29	6.38	−6.51	−6.16	−6.46	0.05
2,3,4,5-Tetrachlorobiphenyl	364	6.41	6.51	−7.16	−6.37	−6.67	0.49
2,3′,4,4′-Tetrachlorobiphenyl	401	5.90	6.51	−7.80	−6.74	−7.04	0.76
2,3′,4′5-Tetrachlorobiphenyl	377	6.39	6.51	−7.25	−5.77	−6.07	1.18
2,2′,3,5′-Tetrachlorobiphenyl	320	6.00	6.26	−6.47	−5.68	−5.98	0.49
2,2′,4,5-Tetrachlorobiphenyl	337	6.10	6.38	−6.57	−5.97	−6.27	0.30
2,2′,5,5′-Tetrachlorobiphenyl	360	6.10	6.38	−7.00	−6.20	−6.50	0.50
3,3′,4,4′-Tetrachlorobiphenyl	453	6.63	6.64	−8.53	−7.39	−7.69	0.84
2,2′,5,6′-Tetrachlorobiphenyl	376	5.50	6.13	−6.80	−6.11	−6.41	0.39
2,2′,6,6′-Tetrachlorobiphenyl	471	5.48	5.88	−8.03	−6.81	−7.11	0.92
2,4,4′,6-Tetrachlorobiphenyl	366		6.38	−6.94	−6.26	−6.56	0.38
3,3′,5,5′-Tetrachlorobiphenyl	437	6.85	6.88	−8.54	−7.47	−7.77	0.77
2,3,7,8-Tetrachlorodibenzofuran	500	6.53	6.70	−8.86	−7.92	−8.22	0.64
1,2,3,4-Tetrachlorodibenzo-p-dioxin	463	7.18	7.31	−8.77	−8.16	−8.46	0.31
1,2,3,7-Tetrachlorodibenzo-p-dioxin	448	8.22	7.31	−8.89	−8.01	−8.31	0.58
1,3,6,8-Tetrachlorodibenzo-p-dioxin	492	6.29	7.55	−9.00	−8.69	−8.99	0.01
2,3,7,8-Tetrachlorodibenzo-p-dioxin	578	6.42	7.31	−10.22	−9.31	−9.61	0.61
2,2′,4,4′-Tetrachlorodiphenylether	342		6.97	−6.82	−6.61	−6.91	−0.09
3,3′,4,4′-Tetrachlorodiphenylether	343		7.05	−6.98	−6.70	−7.00	−0.02
1,1,2,2-Tetrachloroethane	298	2.62	2.64	−1.74	−1.84	−2.14	−0.40
1,1,1,2-Tetrachloroethane	298		3.03	−2.18	−2.23	−2.53	−0.35
1,1,2,2-Tetrachloroethane	298	2.62	2.64	−1.75	−1.84	−2.14	−0.39
Tetrachloroethylene	298	3.40	3.48	−2.54	−2.68	−2.98	−0.44
Tetrachloroethylene	251	3.40	3.48	−2.74	−2.68	−2.98	−0.24
Tetrachloromethane	298	2.83	2.88	−2.31	−2.08	−2.38	−0.07
3,4,5,6-Tetrachloroveratrole	363		4.38	−5.24	−4.23	−4.53	0.71
1,2,4,5-Tetraflurobenzene	277		2.71	−2.38	−1.91	−2.21	0.17
Tetrahydrofuran	298	0.46	0.47	1.15	0.33	0.03	−1.12
Tetrahydropyran	298	0.95	0.88	−0.03	−0.08	−0.38	−0.35
1,2,4,5-Tetramethylbenzene	353	4.00	4.01	−4.59	−3.79	−4.09	0.50
Toluene	178	2.73	2.64	−2.21	−1.84	−2.14	0.07
Triallate	302		4.53	−4.88	−3.77	−4.07	0.81
Triamcinolone	543	1.16	0.93	−3.68	−2.58	−2.88	0.80
1,2,3-Tribromobenzene	361		4.33	−5.07	−4.16	−4.46	0.61
1,2,4-Tribromobenzene	314		4.53	−4.50	−3.89	−4.19	0.31
1,3,5-Tribromobenzene	394	4.51	4.73	−5.60	−4.89	−5.19	0.41
2,4,6-Tribromobiphenyl	339	6.03	6.02	−7.30	−5.63	−5.93	1.37
Tribromomethane	298	2.67	2.37	−1.91	−1.57	−1.87	0.04
2,2,2-Trichloro-1,1-ethanediol	330	0.99	0.71	0.72	−0.23	−0.53	−1.25

Appendix (*Continued*)

Name	T_m(K)	MLOGP	CLOGP	Observed log S_w	Predicted log S_w (OLD)	Predicted log S_w (REV)	Difference
2,3,4-Trichloroanisole	343	4.03	4.11	− 4.29	− 3.76	− 4.06	0.23
2,4,6-Trichloroanisole	334	4.04	4.07	− 4.20	− 3.63	− 3.93	0.27
1,2,3-Trichlorobenzene	326	4.11	4.04	− 4.10	− 3.52	− 3.82	0.28
1,2,4-Trichlorobenzene	289	3.97	4.16	− 3.61	− 3.36	− 3.66	− 0.05
1,3,5-Trichlorobenzene	336	4.17	4.28	− 4.60	− 3.86	− 4.16	0.44
3,4,4′-Trichlorobiphenyl	361	5.90	6.05	− 7.06	− 5.88	− 6.18	0.88
2,5-Trichlorobiphenyl	317	5.60	5.67	− 6.02	− 5.06	− 5.36	0.66
2,3′,5-Trichlorobiphenyl	313	5.76	5.92	− 6.01	− 5.27	− 5.57	0.44
2,4′,-Trichlorobiphenyl	340	5.79	5.92	− 6.25	− 5.54	− 5.84	0.41
2,3,4′,-Trichlorobiphenyl	342	5.42	5.80	− 6.26	− 5.44	− 5.74	0.52
2,4,5-Trichlorobiphenyl	349	5.90	5.92	− 6.27	− 5.63	− 5.93	0.34
2,3,6-Trichlorobiphenyl	322	5.67	5.67	− 6.29	− 5.11	− 5.41	0.88
2,4,6-Trichlorobiphenyl	336	5.60	5.67	− 6.14	− 5.25	− 5.55	0.60
2′,3,4-Trichlorobiphenyl	333	5.87	5.80	− 6.29	− 5.35	− 5.65	0.64
2,4,4′-Trichlorobiphenyl	330	5.80	5.92	− 6.21	− 5.44	− 5.74	0.47
1,2,4-Trichlorodibenzo-*p*-dioxin	402	7.47	6.71	− 7.58	− 6.95	− 7.25	0.33
2,4,5-Trichlorodiphenylether	334		6.29	− 6.58	− 5.85	− 6.15	0.43
3,4,5-Trichlorodiphenylether	327		6.33	− 6.77	− 5.82	− 6.12	0.65
1,1,1-Trichloroethane	298	2.48	2.49	− 2.00	− 1.69	− 1.99	0.01
1,1,2-Trichloroethane	298	2.07	2.05	− 1.48	− 1.25	− 1.55	− 0.07
1,1,1-Trichloroethane	298	2.49	2.48	− 2.14	− 1.68	− 1.98	0.16
Trichloroethylene	298	2.61	2.63	− 1.96	− 1.83	− 2.13	− 0.17
Trichloroethylene	298	2.61	2.63	− 1.93	− 1.83	− 2.13	− 0.20
1,1,2-Trichlorofluoroethane	298		2.20	− 3.04	− 1.40	− 1.70	1.34
Trichloromethane	298	1.97	1.95	− 1.17	− 1.15	− 1.45	− 0.28
1,2,3-Trichloropropane	298		1.98	− 1.92	− 1.18	− 1.48	0.44
3,4,5-Trichloroveratrole	339		3.67	− 4.37	− 3.28	− 3.58	0.79
1,1,1,-Trifluoro-2-propanol	298	0.73	0.81	0.30	− 0.01	− 0.31	− 0.61
2,3,3-Trimethyl-2-butanol	356		1.80	− 0.72	− 1.58	− 1.88	− 1.16
2,2,3-Trimethyl-3-pentanol	298		2.86	− 1.27	− 2.06	− 2.36	− 1.09
1,2,3,-Trimethylbenzene	248	3.59	3.54	− 3.20	− 2.74	− 3.04	0.16
1,2,4-Trimethylbenzene	229	3.63	3.59	− 3.31	− 2.79	− 3.09	0.22
1,3,5-Trimethylbenzene	228	3.58	3.64	− 3.40	− 2.84	− 3.14	0.26
2,2,4-Trimethylpentane	298		4.54	− 4.74	− 3.74	− 4.04	0.70
Triphenylene	472	5.49	5.66	− 6.74	− 6.60	− 6.90	− 0.16
Urea	405	− 2.11	− 2.11	0.96	1.84	1.54	0.58
Veleraldehyde	298		1.23	− 0.85	− 0.43	− 0.73	0.12
Veratrole	298	1.60	1.60	− 1.31	− 0.80	− 1.10	0.21
Vernolate	298	3.84	3.74	− 3.30	− 2.94	− 3.24	0.06
Warfarin	434	2.70	2.44	− 3.89	− 3.00	− 3.30	0.59

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