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Comparison of aqueous solubility estimation from AQUAFAC and the GSE

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ABSTRACT

The GSE (General Solubility Equation) and AQUAFAC (Aqueous Functional Group Activity Coefficients) are two empirical models for aqueous solubility prediction. This study compares the aqueous solubility estimation of a set of 1642 pharmaceutically and environmentally related compounds, using the two methods. The average absolute errors in the solubility prediction are 0.543 log units for AQUAFAC and 0.576 log units for the GSE. About 88.0% of the AQUAFAC solubilities and 83.0% of the GSE molar aqueous solubilities are predicted within one log unit of the observed values. The marginally greater accuracy of AQUAFAC is due to the fact that it utilizes fitted-parameters for many structural fragments and is based on experimental solubility data. The GSE on the other hand is a simpler, non-regression based equation which uses two parameters for solubility prediction.

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1. Introduction

Aqueous solubility is of fundamental importance in a large number of scientific disciplines and practical applications. It helps us understand the drug behavior in an aqueous environment. Therefore, it is essential to have an accurate means for predicting aqueous solubility. The GSE (General Solubility Equation) and the AQUAFAC (Aqueous Functional Group Activity Coefficients) are two such empirical models for aqueous solubility prediction.

The GSE (Jain and Yalkowsky, 2001; Ran et al., 2002) is based on the fact that the aqueous solubility of a solute depends upon its crystallinity and its polarity, which are determined by the melting point (MP) in Celsius, and the octanol–water partition coefficient (ClogP or $\log K_{ow}$), respectively, using the following expression:

$$\log S_w = 0.5 - 0.01(\mathrm{MP} - 25) - \log K_{ow} \quad (1)$$

where, S_w is the molar aqueous solubility. If the solute has a melting point less than 25 °C, i.e., if it is a liquid, the term (MP − 25) is set to zero. The following assumptions are used in the derivation of the GSE for non-electrolyte compounds:

1. The melting point of the solute does not change in the presence of water.
2. The ideal solubility (or the crystal–liquid solubility ratio) of a solid solute is described by the van't Hoff equation, with the entropy of melting being described by the Walden's rule (entropy of melting, $\Delta S_m = 56.7$ J/mol K). This is applicable to most uncharged organic molecules.
3. The heat capacity of melting (Cp_m) is negligible.
4. The effect of mutual saturation of water and octanol is negligible.
5. Organic non-electrolyte liquids are completely miscible with octanol so that the mole fraction is 0.5 (i.e., a molar solubility of 3.15). The logarithm of 3.15 is approximately 0.5, which is the intercept in the GSE.
6. The solubility of the solute is low enough so that the molarity of water is close to 55.5 M.

It should be noted that the GSE is strictly applicable to the non-electrolytes and that no fitted-parameters are used in its derivation.

On the other hand, AQUAFAC model, originally developed by Myrdal et al., is based on group contribution values (q-values) which are based on experimental aqueous solubilities (Myrdal et al., 1992, 1993, 1995; Pinsuwan et al., 1997). The aqueous activity coefficient of a compound is determined using a summation of simple additive constitutive group values, i.e.,

$$\log \gamma_w = \sum n_i q_i \quad (2)$$

where n_i is the number of times group i appears in the compound and q_i is the contribution of group i to the total activity coefficient.

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Table 1
Results of aqueous solubility estimations

	GSE (predicted)	AQUAFAC (fitted)
N	1642	1642
Intercept	−0.259	−0.146
AAE (log unit)	0.576	0.465
RMSE (log unit)	0.773	0.653
Slope	0.867	0.949
R^2	0.882	0.912
Error ≤1 log unit	83.19%	88.06%

N, total number of compounds; AAE, average absolute error; RMSE, root mean-square error; Intercept, slope and R^2 for the plot between experimental and predicted, log molar aqueous solubilities.

The molar aqueous solubility (S_w) for poorly soluble solutes at high dilution can be calculated using

$$S_w = \frac{X_i^c}{\gamma_w} \cdot 55.5 \quad (3)$$

where, X_i^c is the ideal crystalline mole fraction solubility, γ_w is the aqueous activity coefficient and 55.5 mol/L is the molarity of water. Eq. (3) can be combined with the Van't Hoff equation to give

$$\log S_w = 1.74 - \log \gamma_w - \frac{\Delta S_m (T_m - T)}{2.303 \cdot R \cdot T} \quad (4)$$

where, R is the gas constant, ΔS_m is the entropy of melting, T_m is the melting point and T is the ambient temperature, both in Kelvin. Thus, the aqueous solubility can be determined using Eq. (4) where, γ_w is obtained from the AQUAFAC model.

The entropy of melting is calculated using the following equation developed by Dannenfelser and Yalkowsky (1999) and revised by Jain et al. (2004):

$$\Delta S_m = 50 - R \ln \phi + R \ln \sigma \quad (5)$$

where, σ is the molecular symmetry number (the number of positions into which a molecule can be rotated that are identical to a reference position) which accounts for the likelihood of the molecule being in the proper orientation. The molecular flexibility (ϕ) accounts for the likelihood of the molecule being in the proper conformation, for incorporation into the crystal lattice. It is calculated using the following equation:

$$\phi = 2.435^{[SP3+0.5\cdot SP2+0.5\cdot RR-1]} \quad (6)$$

where SP3 is the number of nonring, nonterminal sp^3 atoms like CH_2, CH, C, NH, N, O, S, etc., SP2 is the number of nonring, nonterminal sp^2 atoms like =CH, =C, =N, etc. and RR is the number of rigid single or fused conjugated aromatic ring systems.

In this study we compare aqueous solubilities determined from the GSE and the AQUAFAC model, for 1642 organic compounds.

2. Methods

2.1. Data collection

The experimental molar aqueous solubilities of 1642 pharmaceutically and environmentally related organic compounds were collected from WATERNT™ v 1.0 EPA and AQUASOL databases. The experimental entropies of melting were obtained from Chickos et al., 1999. Eq. (5) was used to calculate the entropies of the compounds for which the experimental values are not available. The calculated partition coefficients for all the compounds were obtained from ClogP software. The melting point data was collected from several electronic and print literature (Merck Index; Chemfinder website; AQUASOL database; EPI Suite, 2000; Howard and Meylan, 1997; Chickos and Nichols, 2002; Jain and Yalkowsky, 2006).

2.2. Solubility prediction

Compounds with observed solubilities of greater than 1 M are not included in the study owing to the fact that the solvent cannot be regarded as pure water. Also, long chain compounds with a flexibility number of 15 or greater are not included due to the possibility of self-association.

2.2.1. GSE

The partition coefficients and the melting points were used to calculate the predicted aqueous solubility using the GSE, Eq. (1).

2.2.2. AQUAFAC

All compounds were fragmented using the group breakdown scheme of Jain and Yalkowsky, 2006, into 147 groups. The predicted aqueous activity coefficients (γ_w) and the entropies of melting (ΔS_m) values were calculated using Eqs. (2) and (5), respectively. AQUAFAC-predicted aqueous molar solubility data (S_w) were calculated from the melting point (MP) and entropy of melting parameters (σ and Φ) and group activity coefficients (γ_w) using Eq. (4). The latter are based on the experimental solubility data.

A ten-fold cross-validation experiment was performed on the complete data set. For each validation, approximately 1/10th of the data were randomly selected using the RAND function, from Microsoft Excel 2000, and used as the test set. The remaining data were used as the training set to generate the group contribution values. Each compound was included in only one test set.

2.3. Statistical analysis

The group contribution values for calculating aqueous activity coefficients were generated by multiple linear regressions using SPSS (version 10.0). All other data analysis was performed using Microsoft Excel (2002). The average absolute error (AAE) for each calculation was determined by

$$AAE = \frac{\sum |\log S_{pred} - \log S_{exp}|}{N} \quad (7)$$

The root mean-square error (RMSE) was determined by

$$RMSE = \sqrt{\frac{\sum (\log S_{pred} - \log S_{exp})^2}{N}} \quad (8)$$

where, $\log S_{pred}$ and $\log S_{exp}$ are the logarithms of molar solubilities, predicted and experimental, respectively, and N is the total number of organic compounds.

3. Results and discussion

A complete alphabetical list of 1642 organic compounds along with their melting points, partition coefficients, experimental as well as AQUAFAC- and GSE-predicted aqueous molar solubility values, is provided in Appendix A. The compounds range from 10^{-13} to 10^{0}, in experimental molar solubility.

Fig. 1 shows the relationship between the experimental and the GSE-predicted aqueous solubilities. As shown in Table 1, the regression line has a slope of 0.867 and an R^2 of 0.882. The AAE in the prediction of aqueous solubilities using the GSE for all the 1642 compounds was observed to be 0.576 log units.

On the other hand, the plot of the experimental versus the AQUAFAC-fitted aqueous solubilities, for 1642 organic compounds

Table 2
Ten-fold cross-validation of the AQUAFAC model

Cross-validation	Training set (fitted)		Test set (predicted)	
	Number of compounds	Average absolute error	Number of compounds	Average absolute error
Round 1	1478	0.464	164	0.541
Round 2	1478	0.468	164	0.503
Round 3	1478	0.466	164	0.506
Round 4	1478	0.467	164	0.554
Round 5	1478	0.463	164	0.515
Round 6	1478	0.453	164	0.587
Round 7	1478	0.457	164	0.600
Round 8	1478	0.470	164	0.447
Round 9	1478	0.462	164	0.552
Round 10	1476	0.454	166	0.624
Average		0.462		0.543
Overall	1642	0.465		

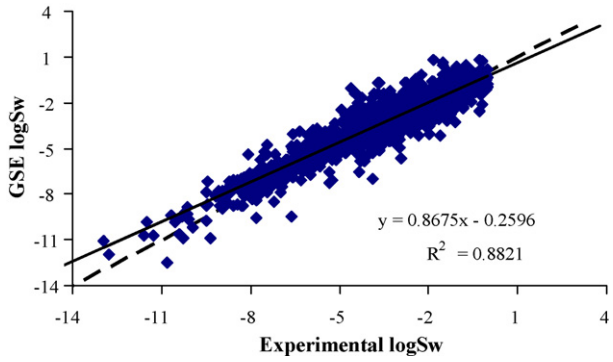

Fig. 1. Plot of logarithm of experimental and GSE-predicted aqueous molar solubilities for 1642 compounds (solid line: regression line; dashed line: line of identity).

(Fig. 2) resulted in a slope of 0.949, an R^2 of 0.912 and an AAE of 0.465 log units (Table 1), which is comparable to the normal error range of solubility data.

The regression line is much closer to the line of identity in Fig. 2 than in Fig. 1, indicating that the estimates from AQUAFAC are closer to the true values than the estimates from the GSE.

Over 88% of the AQUAFAC aqueous solubilities and about 83% of the GSE molar aqueous solubilities are predicted within one log unit of their observed values. These are reasonable estimates considering the size and diversity of the compounds.

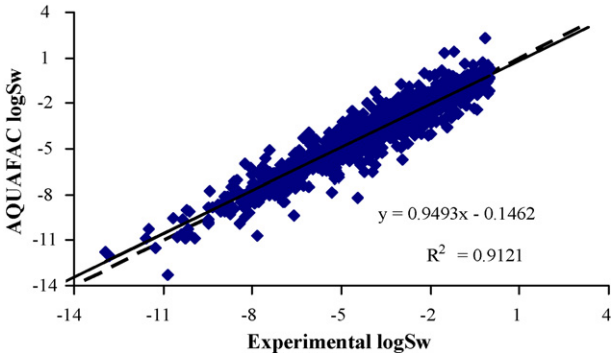

Fig. 2. Plot of logarithm of experimental and AQUAFAC-predicted aqueous molar solubilities for 1642 compounds (solid line: regression line; dashed line: line of identity).

Table 1 summarizes the results of the GSE and AQUAFAC solubility estimation. It is important to realize that a comparison between the GSE and AQUAFAC based on Table 1 is biased, since the training set and the test set in the AQUAFAC model are the same, making it a fitted model, whereas the GSE solubility is purely predicted. Therefore, to compare both the models in a more realistic sense, a ten-fold cross-validation experiment was performed.

The results of the cross-validations are shown in Table 2. The calculated group values from each training set were used to estimate the aqueous solubility of the corresponding training set. The AAE are reported for both the sets.

The mean AAE for the 10 training sets is 0.462 ± 0.006 while the mean AAE for the 10 test sets is 0.543 ± 0.053. The former number is comparable to the overall AAE of 0.465 for the entire data set.

The cross-validation indicates that there is a small increase in the AAE in the test sets when compared to the training sets. This fact is not surprising due to the fact that no outliers were eliminated from the data set. The similarity of the absolute errors for the test and the training sets and the overall average absolute error strongly supports the predictive ability of this method.

The average solubility prediction using AQUAFAC on 10 test sets is 0.543 compared to 0.575 of the GSE. This is a true comparison of the models. Although, both the methods give reasonable solubility predictions, the AQUAFAC model predicts solubilities slightly closer to the true values than the GSE. The marginally improved fit of the AQUAFAC can be explained by the fact that it includes more parameters (MP, σ, Φ and $\sum n_i q_i$) and is based upon experimental aqueous solubility data. The first three parameters give a reasonable estimate of the role of crystallinity in determining solubility. The 147 groups (q_i) account for the wide range of structural variation of nearly 1650 compounds.

The major assumption in the GSE is that the octanol is an ideal solvent for all the solutes. This may not be true for strongly hydrogen bonding compounds, and consequently might result in a larger error for such compounds. However, the GSE is simple, relatively accurate and does not require the use of a training set. Furthermore, it utilizes only two parameters (MP and $\log K_{ow}$) for the solubility determination.

4. Conclusion

The GSE and AQUAFAC models for the prediction of aqueous solubility are compared using a 1642 organic nonelectrolyte data set. Although the GSE is simple and reliable, AQUAFAC model gives a slightly more accurate predicted values.

Appendix A

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
(+)a-(3-Benzoylphenyl)propionic acid	367	3.00	−3.70	−3.19	−2.87
(2,4,5-Trichlorophenoxy)acetic acid	431	3.26	−2.96	−4.09	−4.18
(2,4-Dichlorophenoxy)acetic acid	413	2.62	−2.51	−3.26	−3.21
(4-Chloro-2-methylphenoxy)acetic acid	393	2.52	−2.50	−2.97	−2.61
(4-Chloro-*o*-tolyloxy)acetic acid	393	2.52	−2.50	−2.97	−2.61
(D) 1,2-Diphenyl-1,2-dihydroxyethane	421	2.07	−1.93	−2.79	−3.05
(D) 2-(*m*-Chlorophenoxy)propanoic acid	368	2.39	−2.22	−2.58	−2.20
(D) Methylenebisthiopropionic acid	355	0.56	−1.83	−0.63	−0.17
(Dichloromethyl)benzene	256	3.22	−2.81	−2.72	−2.77
(DL) 1,2-Diphenyl-1,2-dihydroxyethane	393	2.07	−1.93	−2.52	−2.63
(DL) 2-(*m*-Chlorophenoxy)propanoic acid	386	2.39	−2.22	−2.77	−2.54
(DL) 2,3-Dimethylpentane	273	3.63	−4.28	−3.13	−2.91
(DL) 2-Hexanol	273	1.75	−0.87	−1.25	−1.35
(DL) 2-Methyl-3-pentanol	273	1.68	−0.71	−1.18	−1.02
(DL) 3,3-Dimethyl-2-butanol	279	1.64	−0.62	−1.14	−0.93
(DL) 3-Hexanol	273	1.75	−0.80	−1.25	−1.35
(DL) 3-Methyl-2-butanol	273	1.19	−0.20	−0.69	−0.42
(DL) 3-Methylhexane	154	3.71	−4.31	−3.21	−3.23
(DL) 4-Methyl-2-pentanol	183	1.68	−0.79	−1.18	−1.02
(DL) Limonene	273	4.83	−3.99	−4.33	−4.28
(DL) Malathion	276	2.29	−3.36	−1.79	−2.31
(DL) Menthol	301	3.38	−2.50	−2.91	−2.88
(DL) Methylenebisthiopropionic acid	429	0.56	−1.83	−1.37	−1.64
(L) Menthol	316	3.38	−2.50	−3.06	−2.98
1-(4-Chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	351	2.94	−3.61	−2.97	−2.95
1-(Methylamino)-9,10-anthracenedione	443	4.07	−6.30	−5.02	−5.83
1,1-(2,2,2-Trichloroethylidene)bis(4-chlorobenzene)	382	6.79	−7.81	−7.13	−7.52
1,1′-(2,2,2-Trichloroethylidene-bis(4-methoxy)benzene	361	5.67	−6.54	−5.79	−6.32
1,1′-(2,2-Dichloroethylidene)bis(4-ethylbenzene)	332	6.66	−6.49	−6.49	−6.86
1,1′-(2,2-Dichloroethylidenebis(4-chlorobenzene)	382	5.87	−6.55	−6.21	−6.78
1,1,1,2-Tetrachloro-2,2-difluoroethane	314	3.73	−3.31	−3.39	−2.83
1,1,1,2-Tetrachloroethane	203	2.64	−2.20	−2.14	−2.53
1,1,1-Trichloroethane	240	2.68	−2.01	−2.18	−2.21
1,1,1-Trifluoro-*n*-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide	418	4.24	−3.80	−4.94	−5.37
1,1,2,2-Tetrabromoethane	298	3.20	−2.71	−2.70	−2.40
1,1,2,2-Tetrachlorodifluoroethane	300	3.41	−3.23	−2.93	−3.24
1,1,2,2-Tetrachloroethane	231	2.19	−1.77	−1.69	−1.92
1,1,2-Trichloroethane	237	2.01	−2.08	−1.51	−1.74
1,1,2-Trichlorofluoroethane	298	2.62	−3.04	−2.12	−2.40
1,1,2-Trichlorotrifluoroethane	238	3.09	−3.04	−2.59	−3.10
1,1,2-Trifluoro-1,2,2-trichloroethane	237	3.09	−3.04	−2.59	−3.11
1,1,3-Trimethylcyclohexane	207	4.46	−4.85	−3.96	−4.02
1,1,3-Trimethylcyclopentane	131	3.97	−4.48	−3.47	−3.38
1,10-Decanediol	346	2.73	−2.10	−2.70	−3.25
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethylene	360	6.00	−6.90	−6.12	−6.62
1,1-Dichlorobutane	273	2.74	−2.40	−2.24	−2.47
1,1-Dichloroethane	176	1.76	−1.29	−1.26	−1.42
1,1-Dichloroethylene	151	2.12	−1.64	−1.62	−1.97
1,1-Diethoxyethane	173	1.20	−0.43	−0.70	0.02
1,1-Difluoro-1-chloroethane	142	2.05	−1.86	−1.55	−1.95
1,1-Dimethyl-3-phenylurea	405	1.38	−1.61	−1.95	−1.75
1,1′-Ethylidenebis(4-chloro-benzene)	353	6.00	−6.36	−6.05	−6.99
1,2,3,4,6,7,8-Heptachlorodibenzofuran	509	8.23	−11.48	−9.84	−10.30
1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin	538	8.85	−11.25	−10.75	−11.47
1,2,3,4,7,8-Hexachlorodibenzofuran	499	7.92	−10.66	−9.43	−9.58
1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin	546	8.21	−9.95	−10.19	−10.91
1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin	468	7.56	−9.48	−8.76	−9.60
1,2,3,4-Tetrachlorobenzene	320	4.57	−4.56	−4.29	−4.38
1,2,3,4-Tetrachlorodibenzo-*p*-dioxin	458	6.92	−8.77	−8.02	−8.72
1,2,3,4-Tetrahydronaphthalene	237	3.96	−3.47	−3.46	−3.07
1,2,3,4-Tetrahydronaphthlene	237	3.96	−3.45	−3.46	−3.38
1,2,3,5-Tetrachlorobenzene	324	4.57	−4.63	−4.33	−4.44
1,2,3,5-Tetrafluorobenzene	227	2.79	−2.31	−2.29	−2.34
1,2,3,6,7,8-Hexachlorodibenzofuran	506	7.92	−10.33	−9.50	−9.64
1,2,3,6,7,8-Hexahydropyrene	408	6.12	−5.96	−6.72	−6.37
1,2,3,7-Tetrachlorodibenzo-*p*-dioxin	448	6.92	−8.65	−7.92	−8.79
1,2,3,-Trichlorobenzene	326	3.93	−4.08	−3.71	−3.76
1,2,3,-Trimethylbenzene	248	3.63	−3.20	−3.13	−3.08
1,2,3-Tribromobenzene	360	4.66	−5.04	−4.78	−4.82
1,2,3-Trichlorobenzene	327	3.93	−4.00	−3.72	−3.86
1,2,3-Trichloropropane	258	2.50	−1.93	−2.00	−2.08
1,2,3-Trimethylbenzene	248	3.63	−3.20	−3.13	−3.08
1,2,4,5-Tetrabromobenzene	453	5.55	−6.99	−6.60	−6.93

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
1,2,4,5-Tetrachloro-3-nitrobenzene	373	4.39	−5.10	−4.64	−4.98
1,2,4,5-Tetrachlorobenzene	421	4.57	−5.56	−5.30	−5.41
1,2,4,5-Tetrafluorobenzene	277	2.79	−2.38	−2.29	−2.34
1,2,4,5-Tetramethylbenzene	352	4.18	−4.59	−4.22	−4.12
1,2,4-Tribromobenzene	314	4.66	−4.50	−4.32	−4.48
1,2,4-Trichloro-5-((4-chlorophenyl)sulfonyl)benzene	420	5.18	−6.66	−5.90	−7.31
1,2,4-Trichlorobenzene	290	3.93	−3.64	−3.43	−3.54
1,2,4-Trichlorodibenzo-*p*-dioxin	402	6.28	−7.53	−6.82	−7.76
1,2,4-Trimethylbenzene	229	3.63	−3.32	−3.13	−3.08
1,2:3,4-Dibenzanthracene	554	6.70	−8.24	−8.75	−9.49
1,2:5,6-Dibenzanthracene	544	6.70	−8.43	−8.66	−9.87
1,2-Benzacenaphthene	383	4.93	−5.89	−5.28	−5.56
1,2-Benzanthracene	434	5.52	−7.39	−6.38	−7.14
1,2-Benzofluorene	463	5.19	−6.68	−6.34	−6.45
1,2-Benzopyrene	454	6.11	−7.60	−7.17	−7.42
1,2-Bromochlorobenzene	261	3.53	−3.63	−3.03	−3.18
1,2-Chloronitrobenzene	308	2.46	−2.55	−2.06	−2.51
1,2-Dibromo-3-chlorpropane	279	2.68	−2.38	−2.18	−2.32
1,2-Dibromobenzene	275	3.77	−3.50	−3.27	−3.44
1,2-Dibromoethane	283	2.01	−1.68	−1.51	−1.80
1,2-Dibromoethylene	267	1.78	−1.32	−1.28	−2.29
1,2-Dibromopropane	218	2.43	−2.15	−1.93	−2.00
1,2-Dibromotetrafluoroethane	163	2.96	−4.94	−2.46	−3.21
1,2-Dicarbomethoxybenzene	274	1.66	−1.69	−1.16	−1.78
1,2-Dichlorobenzene	257	3.28	−3.26	−2.78	−2.91
1,2-Dichloroethane	237	1.83	−1.29	−1.33	−1.56
1,2-Dichloroethylene	216	1.98	−1.30	−1.48	−1.76
1,2-Dichloropropane	173	2.25	−1.61	−1.75	−1.77
1,2-Dichlorotetrafluoroethane	179	2.78	−2.74	−2.28	−2.97
1,2-Dichloro-tetrafluoroethane	181	2.78	−3.12	−2.28	−2.98
1,2-Dicyanobenzene	414	1.09	−2.51	−1.75	−2.23
1,2-Diethoxyethane	199	0.77	−0.15	−0.27	−0.30
1,2-Diethylbenzene	242	4.07	−3.28	−3.57	−3.63
1,2-Difluorobenzene	226	2.39	−1.00	−1.89	−2.00
1,2-Diiodobenzene	297	4.33	−4.24	−3.83	−4.15
1,2-Diiodoethylene	259	2.63	−3.22	−2.13	−3.00
1,2-Dinitrobenzene	396	1.63	−2.53	−2.11	−2.88
1,2-Diphenylethane	324	4.74	−4.63	−4.50	−4.72
1,2-Propylene oxide	161	0.37	−0.59	0.13	0.07
1,3,5-Tribromobenzene	394	4.66	−5.60	−5.12	−5.93
1,3,5-Trichlorobenzene	337	3.93	−3.78	−3.82	−3.91
1,3,5-Trimethylbenzene	228	3.63	−3.40	−3.13	−3.08
1,3,5-Trinitro-1,3,5-triazacyclohexane	478	0.68	−3.57	−1.98	−3.19
1,3,5-Trinitrobenzene	380	1.45	−2.88	−1.77	−2.65
1,3,6,8-Tetrachlorodibenzo-*p*-dioxin	492	6.92	−9.00	−8.36	−8.98
1,3-Bromochlorobenzene	252	3.53	−3.21	−3.03	−3.18
1,3-Butadiene	164	2.03	−1.87	−1.53	−1.37
1,3-Dibromobenzene	266	3.77	−3.54	−3.27	−3.44
1,3-Dibromopropane	239	2.50	−2.07	−2.00	−2.33
1,3-Dicarbomethoxybenzene	341	1.66	−2.83	−1.59	−2.34
1,3-Dichloro-2-propanol	269	0.78	−0.11	−0.28	−0.32
1,3-Dichlorobenzene	248	3.28	−3.07	−2.78	−2.91
1,3-Dichloropropane	174	2.32	−1.61	−1.82	−2.09
1,3-Difluorobenzene	204	2.39	−2.00	−1.89	−2.00
1,3-Diiodobenzene	307	4.33	−4.57	−3.92	−4.24
1,3-Dimethylnaphthalene	267	4.26	−4.29	−3.76	−4.04
1,3-Dinitrobenzene	363	1.63	−2.50	−1.78	−2.44
1,3-Diphenylurea	512	2.97	−3.15	−4.61	−4.03
1,3-Nitrochlorobenzene	318	2.46	−2.76	−2.15	−2.61
1,4,5-Trimethylnaphthalene	335	4.81	−4.92	−4.68	−4.84
1,4-Bromochlorobenzene	338	3.53	−3.63	−3.43	−3.57
1,4-Bromoiodobenzene	363	4.05	−4.56	−4.20	−4.40
1,4-Cyclohexadiene	224	2.75	−2.06	−2.25	−2.15
1,4-Diamino-2-methoxyanthraquinone	515	3.24	−5.75	−4.91	−5.49
1,4-Diaminoanthraquinone	484	3.16	−5.86	−4.52	−4.39
1,4-Dibromobenzene	360	3.77	−3.95	−3.89	−4.05
1,4-Dicarbomethoxybenzene	414	1.66	−4.01	−2.32	−3.35
1,4-Dichloro-2,5-dimethoxybenzene	404	3.44	−4.41	−4.00	−4.41
1,4-Dichlorobenzene	326	3.28	−3.26	−3.06	−3.19
1,4-Diethylbenzene	230	4.07	−3.75	−3.57	−3.63
1,4-Difluorobenzene	260	2.39	−1.97	−1.89	−2.00
1,4-Dihydroxybenzene	453	1.03	−0.18	−2.08	−0.48
1,4-Diiodobenzene	402	4.33	−5.37	−4.87	−5.17
1,4-Dimethylnaphthalene	280	4.26	−4.14	−3.76	−4.04

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
1,4-Dinitrobenzene	447	1.63	−3.39	−2.62	−3.53
1,4-Nitrochlorobenzene	355	2.46	−2.85	−2.52	−2.74
1,4-Pentadiene	124	2.52	−2.09	−2.02	−2.47
1,5-Dichloro-3-oxapentane	227	1.56	−0.92	−1.06	−1.25
1,5-Dimethylnaphthalene	354	4.26	−4.69	−4.32	−4.48
1,5-Hexadiene	132	3.02	−2.68	−2.52	−2.69
1,8-Dimethylnaphthalene	336	4.26	−4.76	−4.14	−4.36
10H-phenothiazine	458	3.82	−5.10	−4.92	−5.40
11-Alpha-hydroxyprogesterone	438	2.13	−3.82	−3.03	−3.85
13H-dibenzo(*a*,*i*)carbazole	489	5.58	−7.41	−6.99	−7.64
17-Methyltestosterone	438	3.72	−3.95	−4.62	−4.67
1a,2a,3β,4a,5a,6β-Hexachlorocyclohexane	387	4.26	−4.56	−4.65	−5.58
1-Aminoanthraquinone	524	3.53	−5.87	−5.29	−5.44
1-Anthranol	431	3.86	−4.73	−4.69	−4.16
1-Bromo-2-chlorobenzene	261	3.53	−3.19	−3.03	−3.18
1-Bromo-2-chloroethane	256	1.92	−1.32	−1.42	−1.68
1-Bromo-2-ethylbenzene	205	3.92	−3.67	−3.42	−3.54
1-Bromo-2-methylpropane	154	2.58	−2.43	−2.08	−2.09
1-Bromo-3-chloropropane	214	1.85	−1.85	−1.35	−2.21
1-Bromo-3-methylbutane	161	3.07	−2.89	−2.57	−2.62
1-Bromo-4-chlorobenzene	340	3.53	−3.63	−3.45	−3.60
1-Bromobutane	160	2.65	−2.20	−2.15	−2.41
1-Bromoheptane	214	4.12	−4.43	−3.62	−3.99
1-Bromohexane	188	3.63	−3.81	−3.13	−3.46
1-Bromonaphthalene	271	4.06	−4.35	−3.56	−3.99
1-Bromooctane	218	4.61	−5.06	−4.11	−4.51
1-Bromooctane	218	4.61	−5.06	−4.11	−4.51
1-Bromopentane	185	3.14	−3.08	−2.64	−2.94
1-Bromopropane	163	2.16	−1.70	−1.66	−1.89
1-Butene	88	2.17	−2.40	−1.67	−1.81
1-Butyne	147	1.53	−1.28	−1.03	−1.31
1-Chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene	346	6.79	−6.62	−6.77	−7.07
1-Chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene	350	6.00	−6.36	−6.02	−6.53
1-Chloro-2-bromoethane	256	1.92	−1.32	−1.42	−1.68
1-Chloro-2-methylpropane	143	2.49	−2.00	−1.99	−1.97
1-Chlorobutane	150	2.56	−1.93	−2.06	−2.29
1-Chlorodibenzodioxin	378	4.99	−5.72	−5.29	−6.17
1-Chlorodibenzo-*p*-dioxin	371	4.99	−5.72	−5.22	−6.23
1-Chloroheptane	204	4.03	−4.00	−3.53	−3.87
1-Chlorohexane	179	3.54	−3.12	−3.04	−3.34
1-Chloronaphthalene	271	3.81	−3.97	−3.31	−3.72
1-Chloropentane	174	3.05	−2.73	−2.55	−2.82
1-Chloropropane	150	2.07	−1.46	−1.57	−1.77
1-Decanol	280	3.79	−3.63	−3.29	−3.68
1-Decene	207	5.12	−5.39	−4.62	−4.96
1-Ethylnaphthalene	259	4.34	−4.16	−3.84	−4.08
1-Ethyltheobromine	438	0.65	−0.72	−1.55	−1.64
1-Fluoro-4-iodobenzene	246	3.36	−3.13	−2.86	−3.20
1-Heptanethiol	230	3.72	−4.15	−3.22	−3.67
1-Heptanol	240	2.31	−1.81	−1.81	−2.11
1-Heptene	154	3.64	−3.73	−3.14	−3.38
1-Heptyne	192	3.01	−3.01	−2.51	−2.88
1-Hexanol	226	1.82	−1.21	−1.32	−1.58
1-Hexen-3-one	298	1.39	−0.83	−0.89	−0.77
1-Hexene	133	3.15	−3.23	−2.65	−2.86
1-Hexene-3-ol	298	1.61	−0.59	−1.11	−1.25
1-Hexyne	141	2.52	−2.20	−2.02	−2.36
1-Hydroxychlordene	474	4.15	−5.46	−5.41	−4.25
1-Iodobutane	170	3.06	−2.96	−2.56	−2.85
1-Iodoheptane	225	4.54	−4.81	−4.04	−4.43
1-Iodonaphthalene	280	4.34	−4.53	−3.84	−4.34
1-Iodopropane	172	2.57	−2.20	−2.07	−2.33
1-Methyl fluorene	360	4.56	−5.22	−4.68	−5.05
1-Methyl-1-cyclohexene	153	3.51	−3.27	−3.01	−2.65
1-Methylcyclohexene	153	3.51	−3.27	−3.01	−2.65
1-Methylnaphthalene	243	3.72	−3.75	−3.22	−3.57
1-Methylphenanthrene	396	4.89	−5.85	−5.37	−5.86
1-Naphthaleneacetamide	456	1.72	−3.68	−2.79	−3.98
1-Naphthaleneacetic acid	405	2.60	−2.65	−3.17	−3.36
1-Naphthoic acid	435	3.05	−3.30	−3.92	−2.97
1-Naphthyl methylcarbamate	416	2.35	−3.26	−3.03	−3.61
1-Naphthylamine	323	2.25	−1.93	−2.00	−2.54
1-Nitronaphthalene	330	2.99	−4.28	−2.81	−3.52
1-Nonanol	268	3.30	−3.01	−2.80	−3.16

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
1-Nonene	192	4.62	−5.05	−4.12	−4.43
1-Nonyne	223	3.99	−4.24	−3.49	−3.93
1-Octanol	258	2.81	−2.38	−2.31	−2.63
1-Octene	172	4.13	−4.44	−3.63	−3.91
1-Octyne	194	3.50	−3.66	−3.00	−3.41
1-Pentadecanol	317	6.24	−6.35	−5.92	−6.87
1-Pentanethiol	198	2.74	−2.82	−2.24	−2.62
1-Pentanol	196	1.33	−0.60	−0.83	−1.06
1-Pentene	108	2.66	−2.68	−2.16	−2.33
1-Pentyne	183	2.03	−1.64	−1.53	−1.83
1-Phenylethanol	284	1.49	−0.92	−0.99	−1.03
1-Propanethiol	160	1.76	−1.60	−1.26	−1.57
1-Propyl nitrate	173	1.74	−1.50	−1.24	−1.78
1-Tetradecanol	311	5.75	−6.05	−5.38	−6.14
2-(1,3-Dioxolan-2-yl)phenyl methylcarbamate	387	0.25	−1.57	−0.64	−2.07
2-(1′-Cyclohexenyl)cyclohexanone	279	3.73	−2.77	−3.23	−3.46
2-(1-Methylethyl)phenyl methylcarbamate	369	2.37	−2.68	−2.58	−3.18
2-(2,4,5-Trichlorophenoxy)propanoic acid	451	3.68	−3.13	−4.70	−4.82
2-(2,4-Dichlorophenoxy)propanoic acid	389	3.03	−2.83	−3.44	−3.10
2-(3,4-Dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	396	3.22	−5.24	−3.70	−4.24
2-(4-Chloro-2-methylphenoxy)propanoic acid	366	2.94	−2.40	−3.12	−2.55
2-(6-Methoxy-2-naphthyl)propionic acid	439	3.10	−4.16	−4.01	−3.92
2,2,2,*o*,*p*′-Pentachloroethylidenebisbenzene	347	6.79	−6.80	−6.78	−7.07
2,2′,3,3′,4,4′,5,5′,6′-Nonachlorodiphenyl ether	431	9.01	−10.55	−9.84	−10.79
2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl	478	9.56	−10.26	−10.86	−10.86
2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl	429	8.91	−9.47	−9.72	−9.80
2,2′,3,3′,4,4′,5,5′-Octachlorodiphenyl ether	399	8.37	−10.13	−8.88	−9.14
2,2′,3,3′,4,4′,5-Heptachlorodiphenyl ether	377	7.72	−9.12	−8.01	−8.98
2,2′,3,3′,4,4′,6-Heptachlorobiphenyl	395	8.27	−8.30	−8.74	−8.88
2,2′,3,3′,4,4′-Hexachlorobiphenyl	425	7.62	−7.79	−8.39	−8.51
2,2′,3,3′,4,4′-Hexachlorodiphenyl ether	411	7.08	−8.14	−7.71	−8.70
2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl	456	9.56	−10.41	−10.64	−10.65
2,2′,3,3′,4,5,5′6′-Octachlorodiphenyl ether	478	8.37	−10.10	−9.67	−10.63
2,2′,3,3′,4′,5,6-Heptachlorodiphenyl ether	354	7.72	−9.09	−7.78	−8.75
2,2′,3,3′,4,5-Hexachlorobiphenyl	374	7.62	−7.79	−7.88	−8.06
2,2′,3,3′,4-Pentachlorobiphenyl	392	6.98	−7.05	−7.42	−7.59
2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl	434	8.91	−9.47	−9.77	−9.90
2,2′,3,3′,5,5′,6-Heptachlorobiphenyl	395	8.27	−8.59	−8.74	−8.90
2,2′,3,3′,5,5′-Hexachlorobiphenyl	338	7.62	−6.96	−7.52	−7.71
2,2′,3,3′,5′,6-Hexachlorobiphenyl	405	7.62	−7.90	−8.19	−8.33
2,2′,3,3′,6,6′-Hexachlorobiphenyl	385	7.62	−7.90	−7.99	−8.23
2,2′,3,3′-Tetrachlorobiphenyl	394	6.34	−7.28	−6.80	−6.98
2,2′,3,4,4′,5,5′6-Octachlorodiphenyl ether	441	8.37	−10.14	−9.30	−10.26
2,2′,3,4,4′,5,5′-Heptachlorodiphenyl ether	362	7.72	−9.50	−7.86	−8.83
2,2′,3,4,4′,5′,6-Heptachlorobiphenyl	356	8.27	−7.92	−8.35	−8.53
2,2′,3,4,4′,5′-Hexachlorobiphenyl	353	7.62	−7.69	−7.67	−7.88
2,2′,3′,4,4′,5-Hexachlorodiphenyl ether	352	7.08	−8.44	−7.12	−8.10
2,2′,3,4,4′,5′-Hexachlorodiphenyl ether	342	7.08	−8.31	−7.02	−8.00
2,2′,3,4,4′,6′-Hexachlorodiphenyl ether	394	7.08	−8.10	−7.54	−8.01
2,2′,3,4,4′-Pentachlorodiphenyl ether	339	6.43	−7.44	−6.34	−7.34
2,2′,3,4,5,5′,6-Heptachlorobiphenyl	420	8.27	−8.94	−8.99	−9.09
2,2′,3,4′,5,5′,6-Heptachlorobiphenyl	420	8.27	−8.94	−8.99	−9.09
2,2′,3,4′,5,5′,6-Heptachlorodiphenyl ether	391	7.72	−9.05	−8.15	−9.13
2,2′,3,4,5,5′-Hexachlorobiphenyl	358	7.62	−7.68	−7.72	−7.92
2,2′,3,4,5′-Pentachlorobiphenyl	385	6.98	−6.97	−7.35	−7.53
2,2′,3,4,5-Pentachlorobiphenyl	373	6.98	−7.21	−7.23	−7.42
2,2′,3,4,6-Pentachlorobiphenyl	373	6.98	−7.43	−7.23	−7.42
2,2′,3,5,5′,6-Hexachlorobiphenyl	373	7.62	−7.42	−7.87	−8.05
2,2′,3,5′-Tetrachlorobiphenyl	320	6.34	−6.47	−6.06	−6.33
2,2,3-Trimethyl-3-pentanol	298	2.58	−1.27	−2.08	−1.86
2,2′,4,4′,5,5′-Hexachlorobiphenyl	376	7.62	−7.63	−7.90	−8.00
2,2′,4,4′,5,5′-Hexachlorodiphenyl ether	387	7.08	−8.36	−7.47	−8.46
2,2′,4,4′,5,6′-Hexachlorodiphenyl ether	368	7.08	−8.04	−7.28	−7.75
2,2′,4,4′,6,6′-Hexachlorobiphenyl	387	7.62	−8.95	−8.01	−8.10
2,2′,4,4′-Tetrachlorobiphenyl	356	6.34	−6.51	−6.42	−6.64
2,2′,4,4′-Tetrachlorodiphenyl ether	342	5.79	−6.82	−5.73	−6.74
2,2′,4,5,5′-Pentachlorobiphenyl	350	6.98	−7.33	−7.00	−7.25
2,2′,4′,5-Tetrachlorobiphenyl	339	6.34	−7.25	−6.25	−6.63
2,2′,4,5′-Tetrachlorobiphenyl	337	6.34	−6.57	−6.23	−6.48
2,2′,4,6,6′-Pentachlorobiphenyl	358	6.98	−7.32	−7.08	−7.29
2,2,4-Trimethylpentane	166	4.09	−4.67	−3.59	−3.34
2,2′,5,5′-Tetrabromobiphenyl	416	7.32	−8.06	−8.00	−7.99
2,2′,5,5′-Tetrachlorobiphenyl	360	6.34	−6.23	−6.46	−6.62
2,2′,5,6′-Tetrachlorobiphenyl	376	6.34	−6.80	−6.62	−6.82

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
2,2′,5-Trichlorobiphenyl	317	5.69	−5.65	−5.38	−5.67
2,2,5-Trimethylhexane	167	4.58	−5.05	−4.08	−3.87
2,2′,6,6′-Tetrachlorobiphenyl	471	6.34	−7.39	−7.57	−7.65
2,2′-Dichlorobiphenyl	334	5.05	−5.27	−4.91	−5.19
2,2-Dimethyl-1-butanol	298	1.71	−1.04	−1.21	−1.17
2,2-Dimethyl-1-pentanol	298	2.20	−1.52	−1.70	−1.70
2,2-Dimethyl-1-propanol	264	1.22	−0.40	−0.72	−0.65
2,2-Dimethyl-3-pentanol	268	2.13	−1.15	−1.63	−1.46
2,2-Dimethylbutane	174	3.18	−3.67	−2.68	−2.61
2,2-Dimethylpentane	148	3.67	−4.36	−3.17	−3.14
2,2-Dimethylpropane	257	2.69	−3.34	−2.19	−2.09
2,2-Dimethylpropanoic acid	309	1.45	−0.67	−1.06	−0.09
2,3,3′,4,4′,5-Hexachlorobiphenyl	402	7.62	−7.82	−8.16	−8.31
2,3,3′,4,4′,5-Hexachlorodiphenyl ether	408	7.08	−8.78	−7.68	−8.67
2,3,3′,4,4′,6-Hexachlorobiphenyl	380	7.62	−7.66	−7.94	−8.11
2,3,3′,4,4′-Pentachlorodiphenyl ether	338	6.43	−7.67	−6.33	−7.33
2,3,3′,4′,5,6-Hexachlorobiphenyl	395	7.62	−7.83	−8.09	−8.25
2,3,3′4,4′,5,6-Heptachlorodiphenyl ether	442	7.72	−9.46	−8.66	−9.64
2,3,3-Trimethyl-2-butanol	290	2.09	−0.72	−1.59	−1.33
2,3′,4,4′,5,5′-Hexachlorodiphenyl ether	357	7.08	−8.72	−7.17	−8.15
2,3,4,4′,5,6-Hexachlorodiphenyl ether	419	7.08	−8.94	−7.79	−8.78
2,3′,4,4′,5-Pentachlorobiphenyl	382	6.98	−7.39	−7.32	−7.50
2,3′,4,4′-Tetrachlorobiphenyl	401	6.34	−6.89	−6.87	−7.04
2,3,4,5,6-Pentachlorobiphenyl	398	6.98	−7.91	−7.47	−7.70
2,3,4,5-Tetrachloroanisole	361	4.65	−5.26	−4.78	−4.88
2,3,4,5-Tetrachlorobiphenyl	364	6.34	−7.32	−6.50	−6.93
2,3′,4′,5-Tetrachlorobiphenyl	377	6.34	−7.25	−6.63	−6.83
2,3,4,7,8-Pentachlorodibenzofuran	469	6.94	−9.16	−8.15	−8.69
2,3,4-Trichloroanisole	343	4.01	−4.29	−3.96	−4.09
2′,3,4-Trichlorobiphenyl	333	5.69	−6.29	−5.54	−5.81
2,3,4′-Trichlorobiphenyl	342	5.69	−6.26	−5.63	−5.89
2,3,4-Trimethylpentane	164	4.05	−4.70	−3.55	−3.11
2,3,5,6-Tetrachloro-2,5-cyclohexadiene-1,4-dione	567	2.22	−2.99	−4.41	−4.89
2,3′,5-Trichlorobiphenyl	313	5.69	−6.01	−5.34	−5.64
2,3,6-Trichlorobiphenyl	329	5.69	−6.29	−5.50	−5.78
2,3,6-Trichlorophenylacetic acid	432	3.36	−3.08	−4.20	−4.00
2,3,7,8-Tetrachlorodibenzofuran	500	6.29	−8.86	−7.81	−8.12
2,3,7,8-Tetrachlorodibenzo-*p*-dioxin	578	6.92	−10.22	−9.22	−9.03
2,3-Benzofluorene	490	5.19	−8.03	−6.61	−6.67
2,3-Benzofluorene	481	5.19	−7.73	−6.52	−6.77
2,3-Dichloro-1,4-naphthalenedione	469	2.65	−6.36	−3.86	−5.41
2,3-Dichloro-2-methylbutane	298	3.12	−2.69	−2.62	−2.40
2,3-Dichloroanisole	305	3.36	−3.31	−2.93	−3.10
2,3-Dichlorobutane	193	2.67	−2.35	−2.17	−1.97
2,3-Dichlorodibenzo-*p*-dioxin	433	5.63	−7.23	−6.48	−7.26
2,3-Dichlorophenol	330	2.80	−1.66	−2.62	−1.70
2,3-Dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	426	2.30	−2.84	−3.08	−3.64
2,3-Dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	402	1.41	−2.28	−1.94	−2.44
2,3-Dimethyl-1,3-butadiene	197	3.13	−2.40	−2.63	−2.89
2,3-Dimethyl-1-butanol	259	1.64	−0.39	−1.14	−0.90
2,3-Dimethyl-2-butanol	259	1.64	−0.37	−1.14	−0.93
2,3-Dimethyl-3-pentanol	298	2.13	−0.85	−1.63	−1.43
2,3-Dimethylbutane	145	3.14	−3.58	−2.64	−2.38
2,3-Dimethylbutanol	298	1.68	−0.39	−1.18	−0.94
2,3-Dimethylnaphthalene	378	4.26	−4.89	−4.56	−4.63
2,3-Dimethylphenol	346	2.61	−1.43	−2.59	−1.72
2,3-Dinitrotoluene	330	2.18	−2.83	−2.00	−2.67
2,4,4′,6-Tetrachlorobiphenyl	366	6.34	−6.94	−6.52	−6.66
2,4,4′-Trichlorobiphenyl	330	5.69	−6.21	−5.51	−5.79
2,4,4′-Trichlorodiphenyl ether	323	5.14	−6.22	−4.89	−5.92
2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile	526	3.66	−5.65	−5.44	−6.05
2,4,5,6-Tetrachloroanisole	337	4.65	−5.13	−4.54	−4.66
2,4,5-Trichlorobiphenyl	350	5.69	−6.20	−5.70	−6.09
2,4′,5-Trichlorobiphenyl	340	5.69	−6.25	−5.61	−5.87
2,4,5-Trichlorodiphenyl ether	334	5.14	−6.58	−5.00	−6.03
2,4,5-Trichlorophenol	340	3.45	−2.22	−3.37	−2.44
2,4,6-*N*-tetranitroethylaniline	369	2.14	−3.70	−2.35	−4.28
2,4,6-Tribromobiphenyl	339	6.43	−7.30	−6.34	−6.62
2,4,6-Tribromophenol	366	4.18	−3.67	−4.36	−3.18
2,4,6-Trichloroanisole	334	4.01	−4.20	−3.87	−4.00
2,4,6-Trichlorobiphenyl	334	5.69	−6.01	−5.55	−5.82
2,4,6-Trimethyl-1,3,5-trioxane	286	0.70	−0.07	−0.20	−1.36
2,4,6-Trimethylpyridine	229	2.45	−0.54	−1.95	−2.30
2,4,6-Trinitroresorcinol	455	1.06	−1.66	−2.13	−2.30

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
2,4,6-Trinitrotoluene	352	1.99	−3.24	−2.03	−3.12
2,4,6-Tri-*tert*-butylphenol	405	6.39	−3.87	−6.96	−6.03
2,4-Dibromophenol	313	3.29	−2.12	−2.94	−1.99
2,4′-Dichlorobiphenyl	316	5.05	−5.28	−4.73	−5.03
2,4-Dichlorobiphenyl	298	5.05	−5.25	−4.55	−4.88
2,4′-Dichlorodiphenyl ether	304	4.50	−5.52	−4.06	−5.10
2,4-Dichlorophenol	318	2.80	−1.56	−2.50	−1.56
2,4-Dichlorophenyl 4-nitrophenyl ether	342	4.32	−5.45	−4.26	−5.68
2,4-Dimethyl-1-pentanol	298	2.17	−1.60	−1.67	−1.47
2,4-Dimethyl-2-pentanol	298	2.13	−0.92	−1.63	−1.43
2,4-Dimethyl-3-pentanol	298	2.09	−1.22	−1.59	−1.23
2,4-Dimethylpentane	154	3.63	−4.26	−3.13	−2.91
2,4-Dimethylphenol	298	2.61	−1.19	−2.11	−1.21
2,4-Dinitrochlorobenzene	325	2.27	−4.40	−2.04	−2.82
2,4-Dinitrophenol	388	1.73	−1.82	−2.13	−1.75
2,4-Dinitrotoluene	343	2.18	−2.83	−2.13	−2.83
2,4-Octadione	298	1.53	−1.56	−1.03	−1.02
2,5-Dichlorobiphenyl	298	5.05	−5.27	−4.55	−4.88
2,5-Dichlorophenol	331	2.80	−1.91	−2.63	−1.73
2,5-Dimethoxybenzaldehyde	325	1.87	−2.32	−1.64	−2.08
2,5-Dimethylaniline	279	2.17	−1.34	−1.67	−1.84
2,5-Dimethylphenol	348	2.61	−1.54	−2.61	−1.80
2,5-Dinitrophenol	381	1.73	−2.68	−2.06	−1.67
2,6-Dichloro-4-benzenamine	467	2.37	−2.32	−3.56	−4.02
2,6-Dichloro-4-nitroaniline	467	2.76	−4.47	−3.95	−3.97
2,6-Dichloroanisole	304	3.36	−3.10	−2.92	−3.09
2,6-Dichlorobenzonitrile	417	2.83	−3.91	−3.52	−4.02
2,6-Dichlorobenzyl alcohol	370	2.36	−2.10	−2.58	−2.62
2,6-Dichlorobiphenyl	308	5.05	−4.97	−4.65	−4.95
2,6-Dichlorodiphenyl ether	312	4.50	−5.06	−4.14	−5.18
2,6-Dichlorophenol	340	2.80	−1.93	−2.72	−1.63
2,6-Dimethylnaphthalene	383	4.26	−4.89	−4.61	−5.02
2,6-Dimethylphenol	319	2.61	−1.31	−2.32	−1.43
2,6-Dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)benzenamine	321	5.31	−6.26	−5.04	−6.11
2,6-Di-*tert*-butyl-4-methylphenol	344	5.03	−5.56	−4.99	−4.54
2,6-Di-*tert*-butylphenol	311	4.48	−4.92	−4.11	−3.62
2,7-Dichlorodibenzo-*p*-dioxin	474	5.63	−7.83	−6.89	−7.58
2,7-Dimethylnaphthalene	369	4.26	−4.89	−4.47	−4.83
2,8-Dichlorodibenzofuran	457	5.51	−7.21	−6.60	−6.69
2,8-Dichlorodibenzo-*p*-dioxin	424	5.63	−7.18	−6.39	−7.32
2-[(Trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	454	2.84	−5.47	−3.90	−5.40
2-[[3-(Trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	476	4.60	−4.17	−5.88	−5.21
2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	438	2.51	−3.15	−3.41	−3.60
2-Amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	462	−1.52	−1.08	0.38	−0.52
2-Aminobenzoic acid	418	1.36	−1.59	−2.06	−1.23
2-Bromo-2-chloro-1,1,1-trifluoroethane	155	2.26	−1.69	−1.76	−2.44
2-Bromofluorobenzene	298	3.08	−2.70	−2.58	−2.72
2-Bromonaphthalene	329	4.06	−4.40	−3.87	−4.32
2-Bromonaphthalene	329	4.06	−4.40	−3.87	−4.32
2-Bromopropane	184	2.08	−1.59	−1.58	−1.57
2-Bromotoluene	245	3.43	−2.23	−2.93	−3.03
2-Butanethiol	133	2.18	−1.83	−1.68	−1.78
2-Butoxyethanol	198	0.57	−0.42	−0.07	−0.22
2-Butyl benzene	190	3.94	−3.89	−3.44	−3.52
2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	359	5.21	−6.49	−5.32	−7.42
2-Chloro-2-methylbutane	200	2.94	−2.51	−2.44	−2.40
2-Chloro-6-(trichloromethyl)pyridine	338	3.35	−3.51	−3.25	−3.66
2-Chloroanisole	246	2.72	−2.46	−2.22	−2.40
2-Chlorobenzoic acid	413	2.18	−1.87	−2.83	−2.59
2-Chlorobiphenyl	305	4.40	−4.59	−3.97	−4.30
2-Chlorobutane	133	2.49	−1.97	−1.99	−1.97
2-Chlorodibenzodioxin	362	4.99	−5.84	−5.13	−6.03
2-Chlorodibenzo-*p*-dioxin	362	4.99	−5.82	−5.13	−6.15
2-Chlorodiphenyl ether	318	3.85	−4.78	−3.55	−4.61
2-Chloro-*n*-(2,6-diethylphenyl)-*n*-(methoxymethyl)acetamide	316	3.37	−3.05	−3.05	−2.12
2-Chloronaphthalene	332	3.81	−4.14	−3.65	−3.98
2-Chloro-*N*-isopropyl-*N*-phenylacetamide	351	2.42	−2.48	−2.45	−2.15
2-Chloropentane	193	2.98	−2.36	−2.48	−2.50
2-Chlorophenol	283	2.16	−0.65	−1.66	−0.71
2-Chloropropane	156	2.00	−1.40	−1.50	−1.45
2-Cyclohexyl-4,6-dinitrophenol	379	4.54	−4.25	−4.85	−4.38
2-Decanone	287	3.20	−3.31	−2.70	−3.45
2-Ethyl-1,3-hexanediol	233	1.60	−0.54	−1.10	−0.63
2-Ethyl-1-butanol	298	1.75	−1.17	−1.25	−1.27

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
2-Ethyl-1-hexanol	203	2.73	−2.11	−2.23	−2.31
2-Ethyl-2-propanol	264	1.22	−0.20	−0.72	−0.70
2-Ethylanthracene	423	5.38	−6.89	−6.13	−6.69
2-Ethylnaphthalene	266	4.21	−4.29	−3.71	−4.08
2-Ethylphenol	291	2.55	−1.36	−2.05	−1.25
2-Ethylthiophene	298	2.85	−2.59	−2.35	−1.97
2-Ethyltoluene	192	3.58	−3.21	−3.08	−3.12
2-Heptanol	298	2.24	−1.55	−1.74	−1.87
2-Heptanone	238	1.73	−1.42	−1.23	−1.88
2-Hexanone	218	1.24	−0.76	−0.74	−1.35
2-Hexanone	218	1.24	−0.76	−0.74	−1.35
2-Hydroxybenzoic acid	432	2.24	−1.79	−3.08	−0.91
2-Imidazolidinethione	476	−0.49	−0.71	−0.79	−0.30
2-Iodobenzoic acid	435	2.70	−2.73	−3.57	−3.13
2-Iodopropane	183	2.50	−2.08	−2.00	−2.01
2-Isopropoxyphenyl *N*-methylcarbamate	363	1.90	−2.05	−2.05	−2.52
2-Isopropyltoluene	202	4.00	−3.76	−3.50	−3.47
2-Methoxy-4H-1,3,2-benzodioxaphosphorin-2-sulfide	328	2.87	−3.57	−2.67	−2.71
2-Methoxypteridine	423	0.04	−1.11	−0.79	−1.24
2-Methyl pentane	119	3.21	−3.74	−2.71	−2.71
2-Methyl-1,3-butadiene	127	2.58	−2.03	−2.08	−2.13
2-Methyl-1-butanol	273	1.26	−0.47	−0.76	−0.74
2-Methyl-1-butene	136	2.72	−2.73	−2.22	−2.13
2-Methyl-1-pentanol	298	1.75	−1.11	−1.25	−1.27
2-Methyl-1-pentene	137	3.21	−3.03	−2.71	−2.66
2-Methyl-2(methylthio)propionaldehyde *O*-methylcarbamoyloxime	374	1.36	−1.50	−1.62	−1.51
2-Methyl-2-butene	139	2.64	−2.56	−2.14	−1.78
2-Methyl-2-heptanol	223	2.69	−1.72	−2.19	−2.27
2-Methyl-2-hexanol	298	2.20	−1.08	−1.70	−1.75
2-Methyl-2-pentanol	170	1.71	−0.50	−1.21	−1.25
2-Methyl-3-pentanol	298	1.68	−0.70	−1.18	−0.94
2-Methyl-4,6-dinitrophenol	359	2.27	−3.00	−2.38	−1.82
2-Methylanthracene	478	4.89	−6.69	−6.19	−6.58
2-Methylbutane	113	2.72	−3.18	−2.22	−1.88
2-Methylcyclohexanone	298	1.54	−0.94	−1.04	−1.44
2-Methylfuran	182	1.91	−1.44	−1.41	−1.64
2-Methylheptane	168	4.20	−4.48	−3.70	−3.75
2-Methylhexane	155	3.71	−4.60	−3.21	−3.23
2-Methylnaphthalene	308	3.72	−3.76	−3.32	−3.67
2-Methylpentane	120	3.21	−3.79	−2.71	−2.71
2-Methylphenanthrene	330	4.89	−5.84	−4.71	−5.28
2-Methylpropane	135	2.23	−2.55	−1.73	−1.66
2-Methylpropene	133	2.23	−2.33	−1.73	−1.62
2-Naphthoic acid	460	3.05	−3.56	−4.17	−3.33
2-Naphthylamine	386	2.25	−4.35	−2.63	−3.26
2-Nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	365	3.81	−5.22	−3.97	−5.97
2-Nitro-5-methylphenol	303	2.46	−2.75	−2.01	−1.18
2-Nitroaniline	344	2.02	−1.97	−1.98	−1.65
2-Nonanol	238	3.22	−2.74	−2.72	−2.92
2-Nonanone	266	2.71	−2.58	−2.21	−2.93
2-Octanol	242	2.73	−2.09	−2.23	−2.39
2-Octanone	253	2.22	−2.15	−1.72	−2.40
2-Pentanol	200	1.26	−0.30	−0.76	−0.82
2-Pentanol	200	1.26	−0.29	−0.76	−0.82
2-Pentanone	196	0.75	−0.19	−0.25	−0.83
2-Pentanone	196	0.75	−0.30	−0.25	−0.83
2-Pentene	133	2.58	−2.54	−2.08	−1.97
2-Phenoxyethanol	287	1.10	−0.70	−0.60	−0.85
2-Phenyl-3,1-benzoxazin-4-one	397	2.04	−4.61	−2.53	−4.22
2-Phenylethanol	246	1.57	−0.74	−1.07	−1.20
2-*sec*-Butyl-4,6-dinitrophenyl 3-methylcrotonate	341	4.49	−5.51	−4.42	−4.95
2-Undecanol	298	4.21	−2.94	−3.71	−3.97
3-(3,4-Dichlorophenyl)-1,1-dimethylurea	430	2.67	−3.74	−3.49	−3.78
3-(4-Chlorophenyl)-1,1-dimethylurea	448	2.03	−2.94	−3.02	−3.05
3-(5-(1,1-Dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	409	0.34	−1.88	−0.95	−2.13
3(*n*-Octyloxy)-1,2-propanediol	296	2.29	−1.92	−1.79	−1.16
3-(*p*-Tolyl-4-sulfonyl)-1-butyl urea	405	2.41	−3.39	−2.98	−3.39
3,3′,4,4′-Tetrachlorobiphenyl	453	6.34	−8.68	−7.39	−7.49
3,3′,4,4′-Tetrachlorodiphenyl ether	343	6.63	−6.98	−6.58	−6.75
3,3′,5,5′-Tetrachlorobiphenyl	437	6.34	−8.54	−7.23	−7.07
3,3′-Dichlorobiphenyl	302	5.05	−5.80	−4.59	−4.91
3,3-Dimethyl-1-(methylthio)-2-butanone *O*-methylcarbamoyloxime	330	2.16	−1.62	−1.98	−1.77
3,3-Dimethyl-1-butanol	213	1.71	−0.50	−1.21	−1.17
3,3-Dimethyl-2-butanol	279	1.64	−0.62	−1.14	−0.85

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
3,3-Dimethyl-2-butanone	222	1.13	−0.72	−0.63	−0.94
3,3-Dimethylpentane	138	3.67	−4.23	−3.17	−3.14
3,3′-Di-*tert*-butyl-5,5′-dimethyl-2,2-dihydroxydiphenylmethane	404	7.97	−7.23	−8.53	−6.90
3,4,4′-Trichlorobiphenyl	361	5.69	−7.06	−5.82	−6.06
3,4,5,6-Tetrachloroveratrole	363	4.22	−5.24	−4.37	−5.11
3,4,5-Trichlorodiphenyl ether	327	5.98	−6.77	−5.77	−5.96
3,4,5-Trichloroveratrole	339	3.57	−4.37	−3.48	−4.22
3,4-Benzophenanthrene	335	5.52	−8.06	−5.39	−6.28
3,4-Benzopyrene	454	6.11	−8.19	−7.17	−7.91
3,4-Dichloro-2-methoxybenzoic acid	413	2.14	−1.42	−2.78	−3.61
3,4-Dichlorobiphenyl	323	5.05	−7.44	−4.80	−5.10
3,4-Dichloronitrobenzene	314	3.10	−3.20	−2.76	−3.18
3,4-Dichlorophenol	341	2.80	−1.25	−2.73	−1.98
3′,4′-Dichloropropionanilide	364	2.88	−3.16	−3.04	−2.76
3,4-Dimethylisoxazol 5-sulphanylamide	448	1.03	−2.95	−2.03	−2.86
3,4-Dimethylphenol	334	2.61	−1.41	−2.47	−1.55
3,4-Dimethylphenyl methylcarbamate	351	2.27	−2.58	−2.30	−2.56
3,4-Dinitrotoluene	330	2.18	−3.26	−1.99	−2.68
3,5,6-Trichloro-2-pyridinyloxyacetic acid	423	2.53	−2.77	−3.28	−2.95
3,5-Dibromo-4-hydroxybenzonitrile	464	3.39	−3.33	−4.55	−3.49
3,5-Dichlorobenzoic acid	459	3.16	−3.11	−4.27	−3.11
3,5-Dichloro-*N*-(1,1-dimethyl-2-propynyl)benzamide	428	3.57	−4.23	−4.37	−3.89
3,5-Dichlorophenol	341	2.80	−1.48	−2.73	−1.97
3,5-Dimethyl-4-(dimethylamino)phenylmethylcarbamate	362	2.44	−3.35	−2.58	−2.95
3,5-Dimethylphenol	337	2.61	−1.40	−2.50	−1.57
3,5-Dimethylphenyl methylcarbamate	372	2.27	−2.58	−2.51	−2.75
3,5-Dinitrobenzoic acid	480	1.51	−2.20	−2.83	−2.19
3,6-Dichloro-2-methoxybenzoic acid	387	2.14	−1.42	−2.53	−2.82
3-Amino-2,5-dichlorobenzoic acid	476	1.90	−2.47	−3.17	−3.46
3-Aminobenzoic acid	453	0.96	−1.37	−2.01	−0.98
3-Bromo-4-hydroxybenzaldehyde	397	2.12	−2.18	−2.61	−1.91
3-Bromopropylene	154	2.02	−1.50	−1.52	−1.28
3-Chloroanisole	298	2.72	−2.78	−2.22	−2.40
3-Chlorobenzoic acid	427	2.52	−2.54	−3.31	−2.33
3-Chlorobiphenyl	289	4.40	−4.72	−3.90	−4.25
3-Chloropentane	168	2.98	−2.63	−2.48	−2.50
3-Chlorophenol	306	2.16	−0.69	−1.74	−0.96
3-Chloropropionitrile	222	0.60	−0.29	−0.10	−0.64
3-Chloropropylene	139	1.93	−1.36	−1.43	−1.60
3-Ethoxy-4-hydroxybenzaldehyde	351	1.55	−1.77	−1.58	−1.39
3-Ethyl-3-pentanol	261	2.20	−0.85	−1.70	−1.75
3-Heptanol	298	2.24	−1.47	−1.74	−1.87
3-Heptanone	236	1.73	−1.42	−1.23	−1.87
3-Hexanol	298	1.75	−0.80	−1.25	−1.35
3-Hexanone	218	1.24	−0.83	−0.74	−1.34
3-Hexyne	170	2.57	−1.99	−2.07	−2.16
3-Hydroxybenzoic acid	475	1.39	−1.28	−2.66	−0.75
3-Hydroxytoluene	285	2.06	−0.68	−1.56	−0.74
3-Iodobenzoic acid	460	3.04	−3.27	−4.16	−3.46
3-Methyl cholanthrene	452	7.05	−7.92	−8.09	−8.24
3-Methyl-1-butanol	156	1.26	−0.52	−0.76	−0.74
3-Methyl-1-butanol acetate	195	2.26	−1.92	−1.76	−1.64
3-Methyl-1-butene	105	2.59	−2.73	−2.09	−2.16
3-Methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	324	1.96	−2.09	−1.72	−2.31
3-Methyl-2-butanol	298	1.19	−0.20	−0.69	−0.50
3-Methyl-2-butanone	181	0.67	−0.12	−0.17	−0.66
3-Methyl-2-heptanol	298	2.66	−1.72	−2.16	−2.08
3-Methyl-2-pentanol	298	1.68	−0.72	−1.18	−0.94
3-Methyl-2-pentanone	298	1.16	−0.67	−0.66	−1.19
3-Methyl-3-heptanol	190	2.69	−1.60	−2.19	−2.22
3-Methyl-3-hexanol	298	2.20	−1.00	−1.70	−1.75
3-Methyl-3-pentanol	249	1.71	−0.38	−1.21	−1.25
3-Methylacetanilide	339	1.65	−2.09	−1.56	−1.30
3-Methylcyclohexanone	298	1.54	−1.87	−1.04	−1.44
3-Methylheptane	153	4.20	−5.16	−3.70	−3.75
3-Methylindole	368	2.60	−2.42	−2.80	−2.94
3-Methylpentane	110	3.21	−3.68	−2.71	−2.71
3-Methylthiophene	204	2.36	−2.39	−1.86	−1.45
3-Nitroaniline	387	1.47	−2.06	−1.86	−1.96
3-Nitrotoluene	289	2.36	−2.44	−1.86	−2.25
3-Octanol	257	2.73	−1.98	−2.23	−2.39
3-Pentanol	204	1.26	−0.23	−0.76	−0.82
3-Pentanone	234	0.75	−0.25	−0.25	−0.82
3-Pentenenitrile	298	1.11	−0.96	−0.61	−1.15

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
3-Phenyl-1-propanol	273	2.06	−1.38	−1.56	−1.73
3-Phenylpropanol	298	2.06	−1.38	−1.56	−1.73
3-Propyl-2,4-pentadione	298	1.45	−0.88	−0.95	−0.86
4-(1,1-Dimethylethyl)-*n*-(1-methylpropyl)-2,6-dinitrobenzeneamine	339	5.15	−5.47	−5.06	−5.88
4-(2,4,5-Trichlorophenoxy)butanoic acid	387	4.24	−3.83	−4.63	−4.39
4-(2,4-Dichlorophenoxy)butyric acid	391	3.60	−3.73	−4.03	−4.15
4-(4-Chloro-2-methylphenoxy)butanoic acid	373	3.50	−3.68	−3.75	−3.52
4-(4-Chloro-2-methylphenoxy)butanoic acid	373	3.50	−3.68	−3.75	−3.52
4-(4-Nitrophenylazo)aniline	488	3.59	−5.85	−4.99	−5.46
4-(*N*,*N*-dipropylamino)-3,5-dinitrobenzenesulphonamide	415	2.73	−5.14	−3.40	−5.28
4,4′-Dibromobiphenyl	443	5.54	−7.74	−6.49	−6.39
4,4′-Dichlorobiphenyl	422	5.05	−6.56	−5.79	−5.96
4,4′-Dihydroxydiphenyl-2,2-propane	433	3.64	−3.28	−4.49	−4.25
4,4-Dimethyl-1-pentanol	298	2.20	−1.55	−1.70	−1.70
4,5-Dichloroquiaiacol	345	2.63	−2.53	−2.60	−2.08
4,5-Dichloroveratrole	356	2.93	−3.46	−3.01	−3.77
4,6-Dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine	431	3.64	−4.54	−4.47	−3.89
4-Aminoacetophenone	379	0.76	−1.61	−1.07	−1.66
4-Aminobenzoic acid	461	0.96	−1.35	−2.09	−0.97
4-Amino-*N*-(6-methoxy-3-pyridazinyl)benzenesulfonamide	453	0.20	−3.28	−1.25	−2.09
4-Aminopyridine	430	−0.11	−0.05	−0.71	−1.18
4-Bromophenol	336	2.40	−1.09	−2.28	−1.45
4-Bromotoluene	302	3.43	−3.19	−2.97	−3.05
4-Chloroanisole	298	2.72	−2.78	−2.22	−2.40
4-Chloroazobenzene	361	4.76	−5.70	−4.89	−5.40
4-Chlorobenzoic acid	513	2.52	−3.34	−4.17	−3.44
4-Chlorobiphenyl	349	4.40	−5.15	−4.40	−4.59
4-Chlorophenol	316	2.16	−0.73	−1.84	−1.03
4-Chlorophenoxyacetic acid	430	1.97	−2.29	−2.78	−2.81
4-Ethoxy-3-methoxybenzaldehyde	338	1.85	−2.19	−1.75	−2.81
4-Ethyltoluene	211	3.58	−3.11	−3.08	−3.12
4-Heptanol	232	2.24	−1.39	−1.74	−1.87
4-Heptanone	240	1.73	−1.55	−1.23	−1.87
4-Hexylresorcinol	342	4.04	−2.59	−3.97	−2.38
4-Hydroxy-3,5-diiodobenzonitrile	483	3.94	−3.87	−5.29	−4.45
4-Hydroxyazobenzene	425	3.63	−3.34	−4.40	−4.27
4-Hydroxybenzoic acid	488	1.39	−1.44	−2.79	−1.15
4-Hydroxyphenylacetic acid	424	0.95	−0.94	−1.70	−0.97
4-Iodoacetanilide	457	2.27	−3.25	−3.36	−3.26
4-Iodobenzoic acid	544	3.04	−3.96	−5.00	−4.48
4-Isopropyltoluene	205	4.00	−3.77	−3.50	−3.47
4-Methoxybenzoic acid	458	1.96	−2.46	−3.06	−2.29
4-Methoxyphenol	328	1.59	−0.49	−1.39	−0.67
4-Methoxyphenylpropionic acid	377	2.37	−2.21	−2.66	−2.27
4-Methoxypteridine	466	−0.40	−1.11	−0.78	−1.65
4-Methyl-1-pentanol	298	1.75	−1.14	−1.25	−1.27
4-Methyl-1-pentene	120	3.08	−3.24	−2.58	−2.54
4-Methyl-2-pentanol	183	1.68	−0.80	−1.18	−1.02
4-Methyl-2-pentanone	189	1.16	−0.72	−0.66	−1.03
4-Methylbiphenyl	318	4.30	−4.62	−4.00	−4.25
4-Methylcyclohexanol	264	2.05	−0.88	−1.55	−1.49
4-Methyloctane	160	4.69	−6.05	−4.19	−4.28
4-Methylpent-1-ene	119	3.08	−3.24	−2.58	−2.54
4-Methylphenanthrene	325	4.89	−5.85	−4.66	−5.21
4-Methylsulphonyl-2,6-dinitro-*N*,*N*-dipropylaniline	424	2.92	−5.76	−3.68	−5.81
4-Methylthio-3,5-xylyl methylcarbamate	394	2.87	−3.92	−3.33	−3.93
4-Methyoxyacetanilide	404	1.18	−1.30	−1.74	−1.73
4-Nitro-5-methylphenol	401	2.46	−2.11	−2.99	−2.09
4-Nitroaniline	420	1.47	−2.28	−2.19	−2.08
4-Nitrotoluene	325	2.36	−2.49	−2.13	−2.49
4-Oxaheptane	158	2.03	−1.32	−1.53	−1.66
4-Pentene-1-ol	298	1.20	−0.15	−0.70	−0.89
4-*tert*-Butylbenzoic acid	440	3.78	−3.80	−4.70	−3.07
4-*tert*-Butylphenol	373	3.42	−2.41	−3.67	−2.40
5′-(Trifluoromethanesulphonamide)acet-2′,4-xylidide	457	2.72	−3.24	−3.81	−3.62
5,6-Dehydroisoandrosterone acetate	439	3.99	−4.46	−4.90	−5.06
5,6-Dimethylchrysene	401	6.62	−7.01	−7.15	−6.00
5-Bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione	428	1.68	−2.51	−2.48	−2.36
5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	448	1.75	−2.48	−2.75	−1.71
5-Ethylhydantoin	393	−0.23	−0.06	−0.22	0.49
5-Isopropyl-2-methylphenol	274	3.52	−2.08	−3.02	−2.08
5-Isopropyl-*m*-tolyl methylcarbamate	361	3.18	−3.35	−3.31	−3.48
5-Methyl *N*-(methylcarbamoyloxy)thioacetimidate	353	0.61	−0.45	−0.66	−0.39
5-Methyl-1,2,4-triazolo[3,4-*b*]benzothiazole	460	2.48	−2.07	−3.60	−4.09

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
5-Methyl-2-hexanol	298	2.17	−1.38	−1.67	−1.55
5-Methyl-2-hexanone	199	1.66	−1.33	−1.16	−1.56
5-Methylchrysene	390	6.07	−6.59	−6.49	−7.25
5-Nonanone	223	2.71	−2.59	−2.21	−2.92
6-Methyl-2,4-heptadione	298	1.45	−1.60	−0.95	−0.70
6-Methylchrysene	433	6.07	−6.57	−6.92	−7.62
7,8-Benzoquinoline	324	3.32	−3.36	−3.08	−3.94
8-Quinolinol	345	1.66	−2.42	−1.63	−1.32
9,10-Dimethyl-1,2-benzanthracene	396	6.62	−6.83	−7.10	−7.77
9,10-Dimethylanthracene	456	5.44	−6.57	−6.52	−6.54
9-Methylanthracene	352	4.89	−5.89	−4.93	−5.42
Acenaphthalene	363	3.94	−3.96	−4.09	−4.08
Acenaphthene	367	4.15	−4.60	−4.33	−4.24
Acenaphthylene	368	4.15	−3.96	−4.35	−4.08
Acetanilide	388	1.10	−1.33	−1.49	−1.28
Acetohexamide	461	2.44	−1.98	−3.57	−4.00
Acetophenone	293	1.67	−1.29	−1.17	−1.00
Acetylene	192	0.50	−1.34	0.00	−0.45
Acridine	383	3.32	−3.67	−3.67	−4.46
Adenine	636	−0.73	−2.43	−2.15	−1.69
Adipic cid	426	0.23	−0.68	−1.01	−0.73
Adrenosterone	458	1.41	−3.48	−2.51	−2.18
a-Endosulfan	382	3.50	−5.89	−3.84	−5.33
Alachlor	313	3.37	−3.17	−3.02	−3.32
Aldicarb	372	1.36	−1.50	−1.60	−1.78
Aldosterone	437	0.50	−3.85	−1.39	−1.26
Aldoxycarb	414	−0.67	−1.35	0.01	−1.04
Aldrin	377	6.75	−6.31	−7.04	−6.56
Allobarbitiol	443	1.31	−2.06	−2.25	−1.85
Allopurinol	633	−0.55	−2.26	−2.30	−1.04
Allyl bromide	154	2.02	−1.50	−1.52	−1.72
Allyl chloride	139	1.93	−1.36	−1.43	−1.60
Alpha-chlorotoluene	228	2.79	−2.39	−2.29	−2.44
Alpha-estradiol	493	3.94	−5.03	−5.39	−4.56
Alpha-Pinene	211	4.27	−4.74	−3.77	−3.01
Amertryn	357	3.32	−3.04	−3.41	−2.43
a-Methylstyrene	251	3.44	−3.12	−2.94	−3.41
Ametryn	358	3.32	−3.04	−3.42	−3.10
Aminocarb	367	1.90	−2.36	−2.09	−2.78
Amobarbital	429	2.00	−2.57	−2.81	−2.45
Amylacetate	202	2.34	−1.89	−1.84	−1.96
a-Naphthyl acetate	319	2.60	−2.65	−2.31	−2.56
Androstane-17-one	392	4.60	−5.70	−5.04	−5.49
Androstanedione	415	2.55	−3.76	−3.22	−4.40
Androstanolone	454	3.07	−4.16	−4.13	−5.05
Androsterone	458	3.07	−4.40	−4.17	−4.83
Anethole	294	3.39	−3.13	−2.89	−3.21
Aniline	267	1.08	−0.41	−0.58	−0.89
Anisole	236	2.07	−1.85	−1.57	−1.77
Anthracene	489	4.35	−6.61	−5.76	−6.54
Anthraquinone	558	3.34	−5.19	−5.44	−6.43
Aprobarbital	414	1.38	−1.71	−2.04	−1.62
Atrazine	448	2.82	−3.79	−3.82	−3.94
Atropine	389	1.91	−2.12	−2.32	−2.06
Azelaic acid	380	1.70	−1.89	−2.02	−1.71
b(4-Chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	378	2.95	−3.68	−3.25	−3.48
Barban	348	3.41	−4.37	−3.41	−3.31
Barbital	463	0.60	−1.39	−1.74	−0.84
Benazolin	465	2.08	−2.61	−3.25	−1.36
Bendiocarb	403	2.55	−2.93	−3.10	−2.75
Bendroflumethiazide	495	1.82	−3.59	−3.29	−3.59
Benfluralin	339	5.31	−6.53	−5.22	−6.43
Benodanil	410	3.87	−4.21	−4.49	−4.03
Bensulide	307	4.12	−4.20	−3.71	−4.80
Benzaldehyde	247	1.71	−1.19	−1.21	−1.54
Benzaldehyde	216	1.71	−1.21	−1.21	−1.54
Benzamide	402	0.74	−0.95	−1.28	−1.41
Benzamide	402	0.74	−0.95	−1.28	−1.41
Benzene	279	1.99	−1.64	−1.49	−1.66
Benzhydrol	339	2.71	−2.55	−2.62	−2.50
Benzidine	400	1.92	−2.76	−2.44	−2.94
Benzimidazole	443	1.23	−1.77	−2.18	−2.17
Benzo(*a*)fluorene	460	5.19	−6.68	−6.31	−6.58
Benzo(*b*)fluoranthene	440	6.11	−7.79	−7.03	−7.51

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Benzo(*e*)pyrene	451	6.11	−7.80	−7.14	−7.45
Benzo(*g*,*h*,*i*)perylene	551	6.70	−9.02	−8.73	−8.53
Benzo(*j*)fluoranthene	438	6.11	−8.00	−7.01	−7.49
Benzo(*k*)fluoranthene	489	6.11	−8.49	−7.52	−7.75
Benzofluoranthene	424	6.11	−8.23	−6.87	−6.02
Benzoic acid	396	1.87	−1.56	−2.34	−1.22
Benzoin	407	1.84	−2.85	−2.43	−2.65
Benzonitrile	260	1.54	−1.71	−1.04	−1.45
Benzophenone	324	3.15	−3.12	−2.91	−3.14
Benzothiazole	276	2.17	−1.50	−1.67	−1.63
Benzothiophene	305	2.99	−3.01	−2.55	−2.46
Benzotrifluoride	244	2.96	−3.02	−2.46	−3.01
Benzoxazole	303	1.72	−1.15	−1.26	−1.86
Benzyl alcohol	258	1.08	−0.40	−0.58	−0.68
Benzyl alcohol	258	1.08	−0.40	−0.58	−0.68
Benzyl butyl phthalate	298	4.84	−5.64	−4.34	−5.07
Benzyl chloride	228	2.79	−2.38	−2.29	−2.44
Benzylurea	421	0.62	−0.95	−1.35	−0.91
Beta-endosulfan	482	3.50	−6.08	−4.84	−7.50
Betamethasone	503	1.72	−3.77	−3.27	−2.95
Betamethasone-17-valerate	456	3.94	−4.71	−5.02	−5.84
Bibenzyl	323	4.74	−4.62	−4.49	−4.65
Biphenyl	342	3.76	−4.35	−3.69	−4.03
bis-(2-Chloroethyl)-ether	221	1.56	−1.12	−1.06	−1.25
bis-(2-Chloroethyl)-sulfone	329	0.38	−1.50	−0.19	−1.80
bis-(2-Chloroethyl)-sulfoxide	383	0.27	−1.16	−0.62	−1.08
bis-(4-Aminophenyl)methane	364	2.18	−2.30	−2.34	−2.91
Borneol(sp)	479	2.85	−2.32	−4.16	−3.58
Bromazepam	511	1.93	−3.48	−3.56	−3.01
Bromobenzene	242	2.88	−2.55	−2.38	−2.55
Bromochloromethane	185	1.43	−0.89	−0.93	−1.34
Bromocyclohexane	217	3.45	−2.29	−2.95	−2.64
Bromodichloromethane	216	2.09	−1.73	−1.59	−1.34
Bromoethane	155	1.67	−1.09	−1.17	−1.36
Bromomethane	180	1.18	−0.80	−0.68	−0.84
Bromophos	324	5.11	−6.09	−4.87	−5.40
Bromopropylate	349	4.90	−4.93	−4.91	−5.28
Butacarb	376	4.99	−4.24	−5.27	−5.08
Butachlor	270	4.84	−4.19	−4.34	−3.44
Butalbital	412	1.87	−2.12	−2.51	−2.26
Butamben	331	2.78	−3.08	−2.61	−2.99
Butanal	177	0.82	−0.01	−0.32	−0.28
Butane	135	2.31	−2.98	−1.81	−1.98
Butanethiol	157	2.25	−2.18	−1.75	−2.10
Butanoic acid	265	1.07	−0.17	−0.57	0.09
Butethal	400	1.59	−1.83	−2.11	−2.58
Butocarboxim	298	1.21	−0.74	−0.71	−0.64
Buturon	416	2.66	−3.90	−3.34	−3.56
Butyl 4-aminobenzoate	331	2.78	−2.76	−2.61	−2.88
Butyl 9-hydroxy-9H-fluorene-9-carboxylate	344	3.69	−3.89	−3.65	−3.44
Butyl acetate	195	1.85	−1.24	−1.35	−1.44
Butyl acrylate	210	2.20	−1.81	−1.70	−2.02
Butyl alcohol	184	0.84	−0.07	−0.34	−0.53
Butyl benzene	185	4.01	−4.06	−3.51	−3.69
Butyl benzyl phthalate	238	4.84	−5.06	−4.34	−5.07
Butyl butanoate	182	2.83	−2.46	−2.33	−2.47
Butyl ethanoate	195	1.77	−1.14	−1.27	−1.44
Butylate	298	3.85	−3.68	−3.35	−3.72
Butyltoluene	298	4.56	−4.06	−4.06	−4.17
Butyraldehyde	174	0.82	−0.01	−0.32	−0.28
Caffeine	512	0.16	−0.95	−1.80	−0.57
Camphor(sp)	450	3.04	−1.99	−4.06	−3.27
Caproaldehyde	217	1.80	−1.30	−1.30	−1.33
Caprylaldehyde	250	2.78	−2.36	−2.28	−2.38
Carbaryl	418	2.35	−3.26	−3.05	−3.75
Carbazole	516	3.23	−4.97	−4.91	−5.28
Carbendazim	523	1.55	−3.82	−3.30	−2.92
Carbofuran	425	2.30	−2.80	−3.07	−3.89
Carbon tetrabromide	363	2.80	−3.14	−2.95	−3.58
Carbon tetrachloride	249	2.44	−2.29	−1.94	−2.77
Carbon tetrafluoride	90	1.19	−3.67	−0.69	−2.25
Carbophenothion	298	5.19	−5.74	−4.69	−5.67
Carboxin	365	1.49	−3.14	−1.66	−2.92
Carbutamide	417	0.94	−2.71	−1.63	−2.56

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Carvone	298	3.07	−2.06	−2.57	−2.99
Chloralose	456	0.68	−1.84	−1.76	−0.12
Chloramben methyl ester	330	2.60	−3.26	−2.42	−2.53
Chloramphenicol	424	0.92	−2.11	−1.68	−2.84
Chlorbromuron	369	3.15	−3.92	−3.36	−3.69
Chlordane	378	6.26	−5.35	−6.56	−6.51
Chlordene	298	5.68	−5.39	−5.18	−3.95
Chlorflurecol	467	2.88	−4.18	−4.07	−3.76
Chlorimuron	454	2.29	−2.54	−3.35	−4.09
Chloroacetamide	390	−0.58	−0.02	0.16	0.29
Chlorobenzene	228	2.64	−2.38	−2.14	−2.28
Chlorobenzene	228	2.64	−2.35	−2.14	−2.28
Chlorocyclohexane	229	3.36	−2.38	−2.86	−2.52
chlorodibromomethane	253	1.70	−1.90	−1.20	−2.02
Chlorodifluoromethane	116	0.89	−1.49	−0.39	−1.52
Chloroethane	134	1.58	−1.06	−1.08	−1.24
Chloroethane	135	1.58	−0.98	−1.08	−1.25
Chloroethylene	119	1.62	−1.36	−1.12	−1.45
Chloroform	210	1.52	−1.17	−1.02	−1.03
Chloroneb	407	3.44	−4.41	−4.03	−4.32
Chloropham	314	3.30	−3.38	−2.96	−2.52
Chloropropylate	346	4.41	−4.53	−4.39	−5.33
Chlorothalonil	523	3.66	−5.64	−5.41	−5.51
Chlorothiazide	616	−0.23	−3.05	−2.45	−1.76
Chlorotoluron	421	2.58	−3.48	−3.31	−3.20
Chloroxuron	424	4.08	−4.90	−4.84	−5.13
Chlorpropamide	400	2.01	−3.03	−2.53	−3.33
Chlorquinox	463	3.69	−5.43	−4.84	−5.32
Chlorsulfuron	449	2.26	−1.11	−3.27	−2.62
Cholanthrene	446	6.50	−7.85	−7.48	−7.71
Cholesterol	421	8.74	−6.61	−9.47	−9.37
Chrysene	529	5.52	−7.58	−7.33	−7.75
Chrysene	531	5.52	−8.06	−7.35	−8.22
Cinnamic acid	406	2.07	−2.41	−2.65	−1.73
cis-1,2-Dichloroethylene	216	1.98	−1.18	−1.48	−1.76
cis-1,2-Dimethylcyclohexane	223	4.01	−4.33	−3.51	−3.37
cis-1,4-Dimethylcyclohexane	186	4.01	−4.47	−3.51	−3.37
cis-2-Butene	134	2.09	−2.04	−1.59	−1.46
cis-2-Heptene	164	3.56	−3.83	−3.06	−3.02
cis-2-Hexene	132	3.07	−3.23	−2.57	−2.49
cis-2-Pentene	122	2.58	−2.54	−2.08	−1.97
cis-3-Chloro-2-butenoic acid	334	1.35	−0.61	−1.21	−0.33
cis-Crotonic acid	344	0.85	0.00	−0.81	0.38
Citral	298	3.45	−2.06	−2.95	−2.64
Codeine	428	1.28	−1.52	−2.08	−1.70
Coronene	711	7.28	−9.33	−10.90	−8.83
Corticosterone	454	1.99	−3.24	−3.05	−2.74
Cortisone	495	1.81	−3.11	−3.28	−2.42
Cortisone acetate	509	2.14	−4.30	−3.75	−3.54
Cortisone-acetate	508	2.14	−4.00	−3.74	−3.41
Coumaphos	364	4.47	−5.38	−4.63	−5.41
Coumarin	342	1.51	−1.89	−1.45	−1.40
Cyanazine	440	2.51	−3.15	−3.43	−3.14
Cycloate	285	3.81	−3.40	−3.31	−3.54
Cycloheptane	265	3.67	−3.51	−3.17	−2.72
Cycloheptanol	275	2.13	−0.88	−1.63	−1.48
Cycloheptatriene	198	3.02	−2.17	−2.52	−2.82
Cycloheptene	217	3.45	−3.16	−2.95	−2.76
Cyclohexane	280	3.18	−3.18	−2.68	−2.09
Cyclohexanol	297	1.64	−0.38	−1.14	−0.84
Cyclohexanol acetate	208	2.64	−1.67	−2.14	−1.66
Cyclohexanone	245	1.13	−0.59	−0.63	−0.80
Cyclohexene	170	2.96	−2.59	−2.46	−2.12
Cyclooctane	288	4.16	−4.15	−3.66	−3.36
Cyclooctanol	298	2.62	−1.29	−2.12	−0.78
Cyclopentane	180	2.68	−2.65	−2.18	−1.45
Cyclopentene	138	2.47	−2.10	−1.97	−1.48
Cyclopropane	146	1.70	−2.04	−1.20	−0.17
Cyprazine	440	3.12	−3.52	−4.04	−3.02
Dacthal	428	4.24	−5.82	−5.04	−5.85
Daimuron	476	4.30	−5.35	−5.58	−5.19
Danazol	498	3.93	−5.51	−5.43	−6.39
Decachlorobiphenyl	578	10.20	−10.83	−12.50	−13.25
Decachlorodiphenyl ether	494	9.65	−12.95	−11.11	−11.80

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Decalin	243	4.20	−4.35	−3.70	−3.06
Decanoic acid	305	4.02	−3.45	−3.58	−3.16
Delmadinone acetate	442	3.73	−4.95	−4.67	−5.74
Delta-hexachlorocyclohexane	415	4.26	−4.51	−4.93	−5.72
Deoxycorticosterone	414	3.12	−3.74	−3.78	−3.78
Deoxycorticosterone acetate	430	3.71	−4.63	−4.53	−4.90
Desmedipham	393	3.22	−4.63	−3.67	−3.84
Desmetryn	358	2.82	−2.57	−2.92	−2.58
Dexamethasone	539	1.72	−3.77	−3.63	−4.31
Dexamethasone-17-acetate	536	2.46	−4.90	−4.34	−4.78
D-Fenchone	278	3.04	−1.85	−2.54	−1.94
Di(2-ethylhexyl)-phthalate	218	8.39	−6.96	−7.89	−8.48
Diallate	298	4.08	−4.29	−3.58	−4.71
Diallyl phthalate	298	3.36	−3.13	−2.86	−3.54
Diazepam	398	2.70	−3.75	−3.20	−4.35
Diazinon	273	3.86	−3.88	−3.36	−4.21
Dibenz(*a*,*h*)anthracene	539	6.70	−8.74	−8.61	−9.27
Dibenzodioxin	396	4.34	−5.31	−4.82	−5.69
Dibenzofuran	356	3.71	−4.73	−3.79	−4.57
Dibenzofurane	355	4.09	−4.60	−4.16	−3.59
Dibenzo-*p*-dioxin	396	4.34	−5.31	−4.82	−5.01
Dibenzothiophene	371	4.17	−5.10	−4.40	−4.59
Dibromochloromethane	253	2.23	−1.89	−1.73	−1.46
Dibromomethane	221	1.52	−1.17	−1.02	−1.46
Dibutyl ether	178	3.01	−2.64	−2.51	−2.71
Dibutyl phthalate	238	4.61	−4.40	−4.11	−4.92
Dibutylphthalate	238	4.61	−4.40	−4.11	−4.92
Dichlormid	279	2.28	−1.62	−1.78	−1.14
Dichlorodifluoromethane	115	1.82	−1.99	−1.32	−2.50
Dichlorodiphenyldichloroethane	383	5.87	−6.55	−6.22	−6.50
Dichlorodiphenyldichloroethylene	362	6.00	−6.90	−6.14	−6.37
Dichlorodiphenyltrichloroethane	382	6.79	−7.15	−7.13	−6.72
Dichloromethane	178	1.34	−0.82	−0.84	−1.22
Diclofopmethyl	313	4.54	−3.82	−4.19	−5.18
Dieldrin	448	5.45	−6.29	−6.45	−4.32
Diethyl disulfide	172	2.86	−2.61	−2.36	−2.43
Diethyl ether	157	1.05	−0.09	−0.55	−0.61
Diethyl malonate	223	0.90	−0.84	−0.40	−0.66
Diethyl *o*-phthalate	270	2.65	−2.31	−2.15	−2.83
Diethyl phthalate	270	2.65	−2.31	−2.15	−2.83
Diethyl succinate	252	1.39	−0.96	−0.89	−0.87
Diethyl sulfide	169	1.90	−1.46	−1.40	−2.20
Diethylstilbestrol	442	5.64	−4.35	−6.58	−6.04
Difenoxuron	412	3.52	−4.16	−4.16	−4.61
Diflubenzuron	512	3.59	−6.59	−5.23	−6.15
Difluron	504	3.59	−6.02	−5.15	−6.05
Digitoxin	529	2.04	−5.28	−3.85	−5.00
Digoxin	533	0.50	−4.16	−2.35	−4.34
Diiodomethane	279	2.35	−2.51	−1.85	−2.34
Diisobutylphthalate	298	4.46	−4.66	−3.96	−4.29
Diisopropyl ether	186	1.88	−1.06	−1.38	−1.02
Diisopropyl ketone	205	1.58	−1.30	−1.08	−1.53
Diisopropyl sulfide	195	2.74	−2.24	−2.24	−2.61
Diisopropylketone	204	1.58	−1.30	−1.08	−1.53
Dimepiperate	312	4.50	−4.12	−4.14	−3.78
Dimetan	319	1.66	−0.85	−1.37	−1.33
Dimethametryn	338	4.22	−3.71	−4.12	−3.67
Dimethoate	325	0.28	−0.74	−0.05	−0.92
Dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	384	−0.28	−0.33	−0.08	−0.33
Dimethyl carbate	311	1.78	−1.20	−1.41	−1.08
Dimethyl disulfide	188	1.87	−1.44	−1.37	−1.38
Dimethyl fumarate	375	1.21	−0.26	−1.48	−1.02
Dimethyl maleate	254	1.21	−0.26	−0.71	0.25
Dimethyl oxalate	328	−0.58	−0.29	0.79	0.15
Dimethyl phthalate	275	1.66	−1.69	−1.16	−1.78
Dimethyl sulfide	175	0.92	−0.45	−0.42	−1.15
Dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	432	4.24	−5.82	−5.08	−5.93
Dimethylsulfide	175	0.92	−0.45	−0.42	−1.15
Dimethylterephthalate	414	1.66	−4.01	−2.32	−3.17
Di-*n*-butyl succinate	244	3.35	−3.00	−2.85	−2.97
Dinoseb	329	3.67	−3.38	−3.48	−3.88
Diosgenin	468	6.34	−7.32	−7.54	−7.31
Dioxacarb	387	0.25	−1.57	−0.64	−2.18
Diphenamid	408	2.86	−2.98	−3.46	−3.58

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Diphenyl ether	300	4.05	−3.98	−3.57	−3.80
Diphenyl phthalate	345	4.10	−6.59	−4.07	−5.39
Diphenylacetic acid	420	3.06	−3.22	−3.78	−3.80
Diphenylamine	326	3.29	−3.50	−3.07	−3.11
Diphenylcarbinol	339	2.71	−2.55	−2.61	−2.56
Diphenylmethane	298	4.02	−4.08	−3.52	−4.15
Dipropalin	353	4.90	−2.97	−4.95	−5.75
Dipropetryn	378	4.22	−4.20	−4.52	−4.30
Dipropyl ether	147	2.03	−1.62	−1.53	−1.66
Dipropyl sulfide	171	2.88	−2.58	−2.38	−3.25
Disulfoton	381	3.86	−4.23	−4.19	−6.50
Ditolyl ether	298	5.14	−4.85	−4.64	−4.73
Diuron	432	2.67	−3.74	−3.51	−3.48
DL-1,2-Diphenylethanol	340	3.20	−2.52	−3.12	−3.31
D-Limonene	199	4.83	−3.99	−4.33	−4.28
Dodecane	264	6.23	−7.66	−5.73	−6.17
Dodecanedioic acid	403	3.17	−3.76	−3.71	−4.34
Dodecanol	300	4.77	−4.67	−4.29	−4.78
D-Querticol	507	−2.33	−0.17	0.74	2.29
Dulcin	446	1.28	−2.17	−2.26	−1.81
E-3-chloro-2-butenoic acid	334	1.35	−0.61	−1.21	−0.07
Endothall	417	1.89	−0.27	−2.58	0.66
Epiandrosterone	435	3.07	−4.16	−3.94	−4.62
Epichlorohydrin	247	0.63	−0.15	−0.13	−0.25
Epitiostanol	400	4.45	−5.41	−4.97	−5.62
Equilenin	531	3.93	−5.24	−5.76	−5.30
Estradiol	452	3.94	−4.84	−4.98	−4.20
Estragole	298	3.47	−2.92	−2.97	−3.42
Estrone	533	3.43	−3.95	−5.28	−6.51
Ethalfluralin	332	5.23	−6.05	−5.07	−5.89
Ethane	90	1.32	−2.70	−0.82	−0.93
Ethanethiol	125	1.27	−0.60	−0.77	−1.05
Ethinyl-estradiol	415	4.12	−4.30	−4.79	−4.65
Ethiofencarb	307	2.04	−2.09	−1.62	−2.82
Ethiofencarb	307	2.04	−2.09	−1.62	−2.82
Ethion	260	4.75	−5.54	−4.25	−5.71
Ethirimol	431	3.40	−3.02	−4.23	−3.81
Ethisterone	542	3.44	−5.66	−5.38	−6.42
Ethofumesate	343	2.89	−3.42	−2.84	−3.98
Ethoxybenzene	244	2.57	−2.33	−2.07	−2.30
Ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	394	3.22	−4.63	−3.68	−3.67
Ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	310	3.99	−4.40	−3.61	−4.65
Ethyl 4-aminobenzoate	363	1.80	−2.10	−1.95	−2.21
Ethyl acetate	189	0.86	−0.04	−0.36	−0.39
Ethyl acrylate	202	1.22	−0.74	−0.72	−0.97
Ethyl acrylate	202	1.33	−0.82	−0.83	−0.97
Ethyl bromide	154	1.67	−1.08	−1.17	−1.36
Ethyl butyrate	175	1.85	−1.37	−1.35	−1.43
Ethyl caprinate	253	4.79	−4.10	−4.29	−4.57
Ethyl cinnamate	280	2.85	−3.00	−2.35	−0.73
Ethyl cyanoacetate	247	0.02	−0.75	0.48	−0.08
Ethyl heptanoate	207	3.32	−2.74	−2.82	−3.00
Ethyl hexanoate	206	2.83	−2.36	−2.33	−2.49
Ethyl iodide	162	2.08	−1.59	−1.58	−1.80
Ethyl mercaptan	195	1.27	−0.60	−0.77	−1.05
Ethyl *N*-benzoyl-*n*-(3,4-dichlorophenyl)-DL-alaninate	342	4.27	−4.26	−4.21	−5.00
Ethyl nitrate	179	0.45	−0.20	0.05	−0.55
Ethyl pelargonate	236	4.30	−3.80	−3.80	−4.05
Ethyl pentanoate	182	2.30	−1.77	−1.80	−1.95
Ethyl propionate	199	1.36	−0.73	−0.86	−0.90
Ethyl propyl ether	146	1.54	−0.68	−1.04	−1.14
Ethyl valerate	182	2.34	−1.75	−1.84	−1.95
Ethyl vinyl ether	157	0.91	−0.85	−0.41	−1.46
Ethylacetate	190	0.86	−0.02	−0.36	−0.39
Ethylbenzene	178	3.03	−2.80	−2.53	−2.64
Ethylbenzoate	239	2.32	−2.32	−1.82	−2.24
Ethyl-biscoumacetate	450	1.88	−3.66	−2.90	−3.99
Ethylbutyrate	175	1.85	−1.28	−1.35	−1.73
Ethyl-caproate	206	2.83	−2.31	−2.33	−2.47
Ethyl-caprylate	230	3.81	−3.39	−3.31	−3.52
Ethylcyclohexane	161	4.08	−4.25	−3.58	−3.25
Ethylene	104	1.27	−2.33	−0.77	−1.13
Ethyl-isopropyl-ether	298	1.47	−0.55	−0.97	−0.82
Ethynyl estradiol	456	4.12	−4.42	−5.20	−5.01

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Etofenprox	310	7.47	−8.60	−7.09	−7.15
Eucalyptol	309	3.13	−2.49	−2.74	−3.08
Eugenol	266	2.73	−1.56	−2.23	−2.02
Fenbufen	459	3.18	−5.06	−4.29	−3.97
Fenfuram	383	2.62	−3.30	−2.97	−2.48
Fenobucarb	305	2.86	−2.69	−2.43	−2.91
Fenothiocarb	314	3.28	−3.93	−2.94	−3.91
Fenoxycarb	327	4.24	−4.70	−4.03	−4.53
Fensulfothion	298	2.35	−2.30	−1.85	−2.38
Fenthion	281	4.08	−4.57	−3.58	−4.12
Fenuron	406	1.38	−1.61	−1.96	−1.93
Flazasulfuron	441	1.08	−2.29	−2.01	−3.06
Flufenoxuron	444	5.97	−8.09	−6.93	−9.23
Flumethiazide	573	0.09	−0.82	−2.34	−2.11
Fluometuron	437	2.35	−3.32	−3.24	−3.63
Fluorene	388	4.02	−4.94	−4.42	−4.42
Fluorobenzene	231	2.19	−1.80	−1.69	−1.83
Fluorodifen	363	3.81	−5.22	−3.96	−5.45
Fluoromethalone	569	2.06	−4.10	−4.27	−4.85
Fluorotrichloromethane	163	2.13	−2.10	−1.63	−2.64
Flurbiprofen	384	3.81	−4.49	−4.17	−4.29
Fluridone	428	4.48	−4.44	−5.28	−8.21
Flurobenzene	231	2.19	−1.80	−1.69	−1.83
Forchlorfenuron	440	2.42	−3.80	−3.34	−3.04
Furan	188	1.36	−0.82	−0.86	−1.17
Furan	188	1.36	−0.83	−0.86	−1.17
Furfural	235	0.83	−0.10	−0.33	−1.05
Furosemide	479	1.87	−3.66	−3.18	−3.64
Gentisin(sp)	539	3.74	−2.93	−5.65	−3.67
Glyburide	442	4.79	−5.09	−5.73	−6.90
Glyceryl triacetate	275	0.36	−0.58	0.14	0.49
Griseofulvin	493	1.92	−4.60	−3.37	−4.44
Guaiacol	301	1.34	−0.68	−0.87	−0.41
Haloperidol	421	4.20	−5.10	−4.93	−6.72
Halosulfuron	449	0.40	−4.46	−1.41	−2.95
Halothane	155	2.26	−1.71	−1.76	−2.44
Heptabarbital	447	2.79	−3.00	−3.78	−3.59
Heptachlor	368	5.86	−6.32	−6.06	−6.02
Heptachlor-epoxide	433	4.56	−6.05	−5.41	−4.73
Heptanal	229	2.29	−1.96	−1.79	−1.85
Heptane	183	3.78	−4.47	−3.28	−3.55
Heptanoic acid	266	2.54	−1.66	−2.04	−1.49
Heptylbenzene	225	5.49	−5.60	−4.99	−5.27
Hexachloro-1,3-butadiene	252	4.72	−4.92	−4.22	−4.43
Hexachlorobenzene	505	5.86	−7.66	−7.43	−7.15
Hexachlorocyclopentadiene	264	4.63	−5.18	−4.13	−5.15
Hexachloroethane	458	4.03	−3.68	−5.13	−4.99
Hexachloroethane(sp)	460	4.03	−3.67	−5.15	−3.63
Hexadecane	291	8.20	−8.40	−7.70	−8.27
Hexaflumuron	477	5.64	−7.23	−6.93	−8.05
Hexafluoroethane	173	2.15	−4.25	−1.65	−2.72
Hexamethylbenzene	439	5.28	−5.84	−6.19	−5.77
Hexanal	243	1.80	−1.25	−1.30	−1.33
Hexyl acetate	298	2.83	−2.46	−2.33	−2.49
Hexyl ethanoate	212	2.83	−2.45	−2.33	−2.49
Hexyl-4-aminobenzoate	335	3.76	−3.95	−3.63	−4.19
Hexylbenzene	212	5.00	−5.26	−4.50	−4.74
Hydrobenzoin	393	2.07	−1.93	−2.52	−2.38
Hydrochlorothiazide	547	−0.10	−2.62	−1.89	−1.83
Hydrocinnamic acid	321	2.29	−1.41	−2.02	−1.33
Hydrocortisone	485	1.62	−3.05	−2.99	−2.32
Hydrocortisone tebutate	503	4.21	−5.51	−5.76	−5.67
Hydrocortisone-21-acetate	497	2.36	−4.46	−3.85	−3.40
Hydroflumethiazide	544	0.22	−3.04	−2.18	−2.53
Hydroxyisoandrosterone	466	1.93	−3.59	−3.11	−3.65
Hydroxyprogesterone-17alpha	489	3.08	−4.70	−4.49	−4.27
Ibuprofen	349	3.79	−3.76	−3.80	−3.60
Imazosulfuron	456	1.72	−4.79	−2.80	−3.40
Indane	222	3.47	−3.04	−2.97	−2.43
Indazole	420	1.23	−2.16	−1.95	−2.14
Indole	325	2.05	−1.52	−1.82	−2.09
Indoline	298	2.06	−1.04	−1.56	−1.00
Iodobenzene	242	3.16	−2.78	−2.66	−2.90
Iodoethane	162	2.08	−1.60	−1.58	−1.80

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Iodofenphos	345	5.39	−5.31	−5.36	−6.02
Iodomethane	207	1.59	−1.01	−1.09	−1.28
Iorazepam	440	2.41	−3.60	−3.33	−3.00
Ipazine	360	3.86	−3.78	−3.98	−3.97
Isoamyl formate	180	1.72	−1.52	−1.22	−1.47
Isobutane	114	2.23	−3.08	−1.73	−1.66
Isobutene	132	2.23	−2.33	−1.73	−1.62
Isobutyl acetate	174	1.77	−1.21	−1.27	−1.12
Isobutyl formate	177	1.23	−1.00	−0.73	−0.95
Isobutylacetate	212	2.13	−1.21	−1.63	−1.70
Isobutylbenzene	222	3.94	−4.12	−3.44	−3.37
Isobutylformate	177	1.23	−1.01	−0.73	−1.01
Isobutyltoluene	298	4.49	−4.12	−3.99	−4.00
Isoflurane	322	3.00	−1.62	−2.74	−1.51
Isonicotinic acid	593	0.69	−1.37	−3.14	−2.45
Isopentanol	156	1.26	−0.52	−0.76	−0.74
Isopentyl acetate	195	2.26	−1.81	−1.76	−1.64
Isopentyl formate	180	1.72	−1.52	−1.22	−1.47
Isopentyl propionate	200	2.83	−2.25	−2.33	−2.47
Isophorone	265	2.62	−1.06	−2.12	−2.66
Isoprene	127	2.58	−2.03	−2.08	−2.13
Isoprocarb	367	2.37	−2.68	−2.56	−3.17
Isopropyl 4,4′-dibromobenzilate	348	4.90	−6.63	−4.90	−5.84
Isopropyl acetate	200	1.28	−0.52	−0.78	−0.59
Isopropyl ether	188	1.88	−1.06	−1.38	−1.02
Isopropyl formate	193	0.73	−0.63	−0.23	−0.48
Isopropyl methyl ketone	180	0.67	−0.15	−0.17	−0.66
Isopropyl nitrate	191	1.66	−1.46	−1.16	−1.46
Isopropyl phenylcarbamate	360	2.66	−3.00	−2.77	−2.26
Isopropyl *tert*-butyl ether	185	2.34	−2.37	−1.84	−1.45
Isopropylacetate	200	1.28	−0.60	−0.78	−0.59
Isopropylbenzene	177	3.45	−3.29	−2.95	−3.00
Isoproturon	431	2.84	−3.50	−3.67	−3.73
Isoquinoline	300	2.14	−1.46	−1.65	−2.32
Isouron	393	1.51	−2.43	−1.96	−1.90
Ketoprofen	367	3.00	−3.25	−3.19	−2.73
Khellin	427	2.57	−2.40	−3.36	−3.21
L-Carvone	248	3.07	−2.06	−2.57	−2.99
Leptophos	333	6.34	−5.66	−6.19	−6.42
Lidocaine	340	1.66	−1.76	−1.58	−2.11
Linalool	298	3.38	−1.99	−2.88	−2.42
Lindane	386	4.26	−4.43	−4.64	−5.47
Linuron	367	2.91	−3.52	−3.10	−3.40
L-Menthone	267	2.87	−2.49	−2.37	−2.81
Lufenuron	439	6.61	−6.93	−7.52	−8.47
m-Acetotoluidide	339	1.65	−2.09	−1.56	−1.30
Malonic acid diethyl ester	223	0.90	−0.82	−0.40	−0.65
m-Aminophenol	399	0.24	−0.61	−0.75	−0.51
m-Benzenedicarboxylic acid	621	1.76	−3.11	−4.49	−1.73
m-Bromobenzoic acid	428	2.76	−2.70	−3.56	−2.47
m-Bromophenol	306	2.40	−0.88	−1.98	−1.23
m-Bromotoluene	233	3.43	−3.52	−2.93	−3.03
m-Chloroaniline	263	1.72	−1.37	−1.22	−1.52
m-Chlorobromobenzene	252	3.53	−3.21	−3.03	−3.18
m-Chloroiodobenzene	328	3.80	−3.55	−3.60	−3.80
m-Chloronitrobenzene	316	2.46	−2.77	−2.14	−2.56
m-Chlorotoluene	225	3.18	−3.52	−2.68	−2.76
m-Cyanoaniline	326	1.17	−1.17	−0.95	−0.93
m-Cymene	209	4.00	−3.50	−3.50	−3.47
m-Diethylbenzene	189	4.07	−3.75	−3.57	−3.63
Mebendazole	562	2.71	−3.62	−4.85	−4.93
Meconin	375	0.36	−1.89	−0.63	−1.56
Medrogestone	411	4.45	−5.27	−5.08	−6.07
Mefluidide	457	2.72	−3.24	−3.81	−3.44
Megestrol acetate	487	4.00	−5.35	−5.39	−6.04
Menadione	378	2.21	−3.03	−2.51	−2.07
Menthol	315	3.38	−2.54	−3.05	−3.02
Menthone	267	2.87	−2.35	−2.37	−2.81
Meprobamate	378	0.98	−1.67	−1.28	−1.31
Methabenzthiazuron	393	2.65	−3.57	−3.10	−2.32
Methanethiol	150	0.78	−0.49	−0.28	−0.53
Methapyrilene	298	2.55	−2.64	−2.05	−2.29
Methazole	396	3.22	−2.82	−3.70	−3.82
Methiocarb	393	2.87	−3.92	−3.32	−3.84

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Methomyl	351	0.61	−0.45	−0.64	−0.50
Methoprene	437	6.34	−5.34	−7.23	−7.88
Methoxsalen	416	2.30	−3.66	−2.98	−4.35
Methoxybenzene	293	2.07	−2.02	−1.57	−1.77
Methoxychlor	351	5.67	−6.54	−5.70	−6.23
Methoxyflurane	238	2.35	−0.77	−1.85	−0.73
Methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	314	4.54	−5.63	−4.20	−5.21
Methyl 2,4-dichlorophenoxyacetate	315	2.90	−2.96	−2.57	−2.72
Methyl 3-*m*-tolylcarbamoyloxyphenylcarbamate	424	3.27	−4.81	−4.03	−4.28
Methyl 4-aminobenzoate	385	1.31	−1.60	−1.68	−1.84
Methyl 4-hydroxybenzoate	399	2.00	−1.78	−2.50	−1.39
Methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	358	4.15	−5.93	−4.25	−6.00
Methyl acrylate	198	0.73	−0.24	−0.23	−0.44
Methyl benzoate	261	1.83	−1.81	−1.33	−1.72
Methyl butyl ether	158	1.54	−0.99	−1.04	−1.14
Methyl butylketone	218	1.24	−0.80	−0.74	−1.35
Methyl butyrate	187	1.36	−0.83	−0.86	−0.90
Methyl chloride	175	1.09	−0.98	−0.59	−0.72
Methyl decanoate	255	4.30	−4.63	−3.80	−4.05
Methyl hexanoate	202	2.34	−1.99	−1.84	−1.95
Methyl isopropyl ether	127	0.98	−0.06	−0.48	−0.29
Methyl laurate	314	5.28	−4.69	−4.94	−5.46
Methyl methacrylate	225	1.28	−0.82	−0.78	−1.20
Methyl *n*-butyl ether	158	1.54	−0.99	−1.04	−1.14
Methyl nonanoate	273	3.81	−3.88	−3.31	−3.52
Methyl octanoate	233	3.32	−3.39	−2.82	−3.00
Methyl pentanoate	273	1.77	−1.36	−1.27	−1.43
Methyl phenyl ether	236	2.07	−2.02	−1.57	−1.77
Methyl propionate	186	0.86	−0.15	−0.36	−0.38
Methyl propyl ether	134	1.05	−0.39	−0.55	−0.61
Methyl *tert*-butyl ether	165	1.43	−0.24	−0.93	−0.72
Methyl valerate	298	1.85	−1.36	−1.35	−1.43
Methyl-4-aminobenzoate	383	1.31	−1.59	−1.66	−1.80
Methyl-4-methoxybenzoate	323	1.91	−2.41	−1.66	−2.12
Methyl-capronate	202	2.34	−2.00	−1.84	−1.95
Methylcyclohexane	147	3.59	−3.85	−3.09	−2.73
Methylcyclopentane	131	3.10	−3.30	−2.60	−2.09
Methyldymron	345	3.58	−3.35	−3.55	−3.68
Methylphenylsulfide	256	2.59	−2.39	−2.09	−2.39
Methylprednisolone	513	1.82	−3.49	−3.47	−2.60
Methyl-*t*-butyl ether	165	1.43	−0.24	−0.93	−0.72
Metobromuron	369	2.51	−2.89	−2.72	−3.06
Metolachlor	233	3.24	−2.73	−2.74	−2.08
Metolcarb	350	1.72	−1.80	−1.74	−2.01
Metoxuron	400	2.11	−2.53	−2.63	−2.73
m-Fluorobenzoic acid	397	2.07	−1.97	−2.56	−1.48
m-Fluorobromobenzene	298	3.08	−2.67	−2.58	−2.72
m-Hydroxybenzaldehyde	381	1.23	−1.23	−1.56	−0.87
m-Hydroxybenzyl alcohol	346	0.60	−0.27	−0.58	0.26
m-Hydroxytoluene	285	2.06	−0.68	−1.56	−0.74
Mininoxidil	533	1.35	−1.98	−3.20	−1.52
m-Nitrobenzaldehyde	331	1.53	−1.97	−1.36	−1.95
m-Nitrobenzoic acid	414	1.69	−1.67	−2.35	−1.51
m-Nitrobenzyl alcohol	300	0.89	−2.41	−0.41	−0.82
m-Nitrobromobenzene	329	2.70	−1.31	−2.51	−2.94
m-Nitrophenol	371	1.91	−1.01	−2.14	−1.04
Monolinuron	353	2.26	−2.57	−2.31	−2.59
Monuron	444	2.03	−2.94	−2.99	−2.98
m-Terphenyl	360	5.52	−5.18	−5.64	−6.26
m-Toluic acid	382	2.42	−2.14	−2.76	−1.52
m-Toluidine	242	1.62	−0.85	−1.12	−1.36
m-Xylene	225	3.09	−2.82	−2.59	−2.61
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	328	4.82	−6.01	−4.61	−5.69
N-(2-chloroethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzeneamine	318	5.07	−5.60	−4.77	−5.88
N(3),*N*(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	372	3.96	−5.47	−4.20	−5.29
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	396	3.29	−4.43	−3.76	−3.71
N′-(3-chloro-4-methoxyphenyl)-*N*,*N*-dimethylurea	399	2.11	−2.53	−2.62	−2.67
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	353	4.18	−4.45	−4.23	−3.88
N-(4-chlorophenyl)-2,2-dimethylpentanamide	360	4.09	−4.02	−4.21	−3.94
N′-(4-chlorophenyl)-*N*-methoxy-*N*-methylurea	353	2.26	−2.36	−2.31	−2.52
N-(cyclopropylmethyl)-2,6-dinitro-*n*-propyl-4-(trifluoromethyl)benzenamine	306	5.62	−6.54	−5.20	−5.29
N,*N*′-diethylthiourea	349	0.60	−1.46	−0.61	−1.86
N,*N*′-(2-hydroxyethyl)-1,4-diaminoanthraquinone	521	2.71	−5.77	−4.44	−5.17
N,*N*-(2-hydroxyethyl)-4-phenylazoaniline	407	2.75	−3.96	−3.34	−3.98

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
N,*N*-(2-hydroxyethyl)-4-phenylazoaniline	407	2.75	−3.96	−3.34	−3.98
N,*N*-diethyl-2-(1-naphthyloxy)propionamide	345	3.33	−3.57	−3.30	−3.72
N,*N*-dimethyl-2,2-diphenylacetamide	407	2.86	−2.96	−3.45	−3.45
N,*N*-dimethyl-4-phenylazoaniline	389	4.29	−5.99	−4.70	−5.36
N,*N*-dimethylaniline	276	2.17	−1.92	−1.67	−2.13
N,*N*-dimethyl-*N*′-[3-(trifluoromethyl)-phenyl]urea	434	2.35	−3.32	−3.21	−3.69
N,*N*-dimethyl-*N*′-[4-(1-methylethyl)phenyl]urea	431	2.84	−3.50	−3.66	−3.87
N,*N*′-dinitroethanediamine	450	−1.80	−1.81	0.78	−1.81
N,*N*′-di-*n*-propyladipamide	452	1.21	−1.81	−2.25	−3.23
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	432	3.42	−5.40	−4.26	−5.47
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-*N*-phenyl-propanamide	370	3.62	−3.71	−3.84	−3.49
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-*N*,*N*′-dimethylurea	435	1.78	−1.96	−2.65	−2.15
n-Amyl-carbamate	367	1.45	−1.47	−1.64	−1.88
Naphthacene	614	5.52	−8.19	−8.18	−8.10
Naphthalene	353	3.17	−3.62	−3.22	−3.62
Napropamide	348	3.33	−3.57	−3.33	−3.89
n-Butyl benzoate	251	3.30	−3.48	−2.80	−3.22
n-Butyl mercaptan	158	2.25	−2.18	−1.75	−2.10
n-Butylbenzene	185	4.01	−4.06	−3.51	−3.69
N-butyl-*N*′-(3,4-dichlorophenyl)-*N*-methylurea	374	4.15	−4.76	−4.41	−4.51
N-butyl-*N*-ethyl-2,6-dinitro-4-trifluoromethylaniline	339	5.31	−6.53	−5.21	−6.59
n-Decane	244	5.25	−6.44	−4.75	−5.12
Neburon	375	4.15	−4.76	−4.42	−4.71
n-Heptyl carbamate	339	2.44	−2.62	−2.35	−2.34
n-Hexane	178	3.29	−3.96	−2.79	−3.03
n-Hexyl carbamate	335	1.95	−1.92	−1.82	−1.99
Nicosulfuron	415	−1.15	−1.53	0.48	−1.19
Nicotinic acid	510	0.69	−0.84	−2.31	−1.65
Nifedipine	446	2.50	−4.76	−3.48	−5.75
Nitralin	425	2.92	−5.76	−3.69	−6.21
Nitrapyrin	336	3.35	−3.76	−3.23	−1.69
Nitrobenzene	279	1.81	−1.77	−1.31	−1.77
Nitroethane	184	0.45	−0.20	0.05	−0.55
N-methyl-2,4,6,*N*-tetranitroaniline	403	1.64	−3.59	−2.18	−4.13
n-Octane	216	4.27	−5.24	−3.77	−4.08
n-Octylbenzene	234	5.98	−6.46	−5.48	−5.79
Nonanal	254	3.27	−3.17	−2.77	−2.90
Nonane	220	4.76	−6.02	−4.26	−4.60
Nonanoic acid	286	3.52	−2.75	−3.02	−2.54
Norethindrone	479	2.99	−4.63	−4.30	−4.40
Norethindrone acetate	480	3.99	−4.80	−5.31	−5.37
Norethisterone-acetate	434	3.99	−4.79	−4.85	−4.84
Norflurazon	450	2.19	−4.04	−3.21	−4.75
Noscapine	448	1.97	−3.14	−2.97	−2.64
Novaluron	451	5.26	−6.97	−6.29	−6.87
n-Pentadecane	283	7.71	−9.45	−7.21	−7.75
N-phenyl-*N*[1-(2-phenylethyl)-4-piperidinyl]propanamide	357	3.89	−3.23	−3.98	−4.19
n-Propylbenzene	174	3.52	−3.36	−3.02	−3.17
N-sulfanilylsulfanilamide	407	0.09	−2.76	−0.68	−1.92
N-*tert*-butylurea	450	0.27	−0.73	−1.29	−0.92
n-Tridecane	268	6.73	−7.59	−6.23	−6.70
n-Undecane	248	5.74	−7.55	−5.24	−5.65
O-(2-chloro-4-nitrophenyl) *O*,*O*-dimethyl phosphorothioate	324	3.39	−4.31	−3.15	−4.55
O-(4-bromo-2,5-dichlorophenyl) *O*,*O*-dimethyl phosphorothioate	325	5.11	−6.09	−4.88	−6.01
O-(4-bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphonothioate	346	6.34	−7.14	−6.31	−6.75
O,*O*-diethyl *O*-4-nitrophenyl phosphorothioate	278	3.73	−4.42	−3.23	−4.56
O,*O*-diethyl *O*-quinoxalin-2-yl phosphothioate	304	3.04	−4.13	−2.60	−4.40
O,*O*-diethyl-*O*-(3,5,6-trichloro-2-pyridyl)phosphorothioate	315	4.66	−5.50	−4.33	−5.78
O,*O*-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	310	4.12	−4.20	−3.74	−4.62
O,*O*-dimethyl *O*-(2,4,5-trichlorophenyl) phosphorothioate	313	4.86	−5.51	−4.51	−5.44
O,*O*-dimethyl *O*-4-nitrophenyl phosphorothioate	308	2.75	−3.84	−2.35	−3.63
O,*O*-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate	321	0.28	−0.96	−0.01	−0.54
O,*O*-dimethyl-*O*-(3,5,6-trichloro-2-pyridyl)phosphorothioate	319	3.68	−4.83	−3.39	−4.79
o,*p*′-Dichlorodiphenyldichloroethane	349	5.87	−6.51	−5.88	−6.12
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl *O*,*O*-diethyl phosphorothioate	324	3.53	−4.95	−3.29	−5.27
o-Acetoxybenzoic acid	408	1.13	−1.59	−1.73	−1.51
o-Aminophenol	447	0.60	−0.74	−1.59	−1.12
o-Benzenedicarboxylic acid	507	1.07	−1.37	−2.66	−1.80
o-Bromobenzoic acid	423	2.42	−2.03	−3.17	−2.69
o-Bromobenzyl alcohol	353	1.97	−2.16	−2.02	−2.35
o-Chloroacetanilide	361	1.18	−1.40	−1.31	−1.49
o-Chloroaniline	274	1.72	−1.19	−1.22	−1.34
o-Chloroanisole	246	2.72	−2.46	−2.22	−2.40
o-Chlorobiphenyl	307	4.40	−4.54	−3.99	−4.33

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
o-Chloroiodobenzene	274	3.80	−3.54	−3.30	−3.53
o-Chlorotoluene	235	3.18	−2.53	−2.68	−2.76
Octachlorodibenzofuran	531	8.87	−11.59	−10.70	−10.88
Octachlorodibenzo-*p*-dioxin	595	9.50	−12.79	−11.97	−12.00
Octafluorocyclobutane	233	2.29	−3.92	−1.79	−4.02
Octafluoropropane	126	3.12	−4.52	−2.62	−3.39
Octanal	288	2.78	−2.36	−2.28	−2.38
Octanoic acid	290	3.03	−2.26	−2.53	−2.01
o-Cymene	202	4.00	−3.76	−3.50	−3.47
o-Diethylbenzene	242	4.07	−3.28	−3.57	−3.63
O-ethyl *O*-(4-nitrophenyl)-phenylphosphonothioate	308	4.47	−5.02	−4.07	−4.63
o-Ethyltoluene	192	3.58	−3.21	−3.08	−3.12
o-Fluorobenzoic acid	400	1.73	−1.29	−2.25	−1.77
o-Hydroxyacetanilide	365	0.62	−2.23	−0.78	0.01
o-Hydroxybenzamide	412	1.03	−1.82	−1.67	−0.70
o-Hydroxybenzyl alcohol	360	0.60	−0.29	−0.72	−0.40
o-Hydroxybiphenyl	331	3.28	−2.39	−3.10	−2.50
o-Hydroxytoluene	304	2.06	−0.62	−1.62	−0.79
O-isobutyl carbamate	336	0.89	−0.30	−0.77	−0.49
o-Methoxybenzamide	402	0.28	−1.78	−0.82	−1.99
o-Methoxybenzoic acid	374	1.61	−1.48	−1.87	−1.54
o-Methoxyphenol	305	1.34	−0.82	−0.91	−0.26
o-Nitroacetanilide	367	1.07	−1.91	−1.26	−1.49
o-Nitrobenzaldehyde	317	1.53	−1.81	−1.22	−2.09
o-Nitrobenzoic acid	419	1.35	−1.33	−2.06	−2.45
o-Nitrobenzyl alcohol	347	0.89	−1.49	−0.88	−1.74
o-Nitrophenol	318	1.91	−1.75	−1.61	−0.84
o-Nitrotoluene	269	2.36	−2.32	−1.86	−2.25
o-Octyl carbamate	340	2.93	−3.30	−2.85	−3.23
o-Phenylenediamine	374	0.16	−0.43	−0.42	−1.47
Orbencarb	282	3.90	−4.03	−3.40	−4.09
Oryzalin	414	2.73	−3.61	−3.39	−5.30
Osthole	356	3.95	−4.31	−4.03	−5.12
o-Terphenyl	329	5.52	−5.27	−5.33	−5.87
o-Toluic acid	377	2.08	−2.06	−2.37	−1.65
o-Toluidine	288	1.62	−0.81	−1.12	−1.36
o-Tolylurea	464	1.25	−1.82	−2.41	−1.44
Oxasulfuron	431	1.25	−3.89	−2.08	−2.84
Oxazepam	478	2.32	−3.95	−3.62	−2.31
Oxycarboxin	393	1.41	−2.43	−1.86	−2.26
o-Xylene	248	3.09	−3.00	−2.59	−2.61
p-Acetotoluidide	427	1.65	−2.09	−2.44	−2.18
p-Acetoxy-acetanilide	426	0.70	−1.91	−1.48	−1.76
p-Aminobenzene sulphonamide	439	−0.55	−1.36	−0.36	−1.25
p-Aminophenol	463	0.24	−1.26	−1.38	−1.11
p-Benzoquinone	388	0.25	−0.99	−0.65	−1.65
p-Bromobenzoic acid	525	2.76	−3.53	−4.53	−3.09
p-Bromobenzyl alcohol	350	1.97	−2.16	−1.99	−2.06
p-Bromoiodobenzene	363	4.05	−4.56	−4.20	−4.30
p-Bromophenyl urea	500	1.60	−1.63	−3.12	−2.22
p-Bromotoluene	302	3.43	−3.19	−2.97	−3.06
p-Chloroacetanilide	451	1.74	−2.84	−2.77	−2.58
p-Chloroaniline	344	1.72	−1.51	−1.68	−1.88
p-Chloroiodobenzene	326	3.80	−4.03	−3.58	−3.82
p-Chloronitrobenzene	357	2.46	−2.92	−2.55	−2.92
p-Chlorotoluene	281	3.18	−3.08	−2.68	−2.76
p-Chlorotoluene	281	3.18	−3.08	−2.68	−2.76
p-Cyanobenzoic acid	492	1.42	−2.09	−2.86	−1.74
p-Cymene	199	4.00	−3.76	−3.50	−3.47
p-Dichlorobenzene	326	3.28	−3.31	−3.06	−3.10
p-Diethylbenzene	230	4.07	−3.62	−3.57	−3.63
p-Difluorobenzene	260	2.39	−1.97	−1.89	−2.00
Pebulate	251	3.51	−3.31	−3.01	−3.84
Pelletierine	298	0.54	−0.45	−0.04	−0.37
Penbutolol	343	4.20	−1.62	−4.15	−1.62
Pencycuron	403	5.51	−6.04	−6.06	−5.88
Pendimethalin	330	4.82	−6.01	−4.64	−5.19
Pentachlorobenzene	358	5.22	−5.48	−5.32	−5.41
Pentachlorobutadiene	298	4.22	−4.23	−3.72	−3.70
Pentachloroethane	244	3.63	−2.62	−3.13	−2.71
Pentachloronitrobenzene	418	5.03	−5.83	−5.73	−5.85
Pentachlorophenol	463	4.74	−4.28	−5.88	−4.11
Pentaerythrityl tetrabromide	434	4.06	−5.38	−4.91	−5.37
Pentafluorochloroethane	174	2.47	−3.43	−1.97	−2.85

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Pentamethylbenzene	328	4.73	−3.98	−4.53	−4.24
Pentanal	182	1.31	−0.87	−0.81	−0.80
Pentane	144	2.80	−3.28	−2.30	−2.50
Pentanoic acid	240	1.56	−0.63	−1.06	−0.44
Pentyl 4-aminobenzoate	325	3.27	−3.35	−3.04	−3.40
Pentyl acetate	202	2.34	−1.88	−1.84	−1.96
Pentyl propanoate	200	2.83	−2.25	−2.33	−2.47
Pentylbenzene	198	4.50	−4.64	−4.00	−4.22
Pentylcyclopentane	190	5.07	−6.08	−4.57	−3.90
Perchloropropylene	200	6.09	−4.17	−5.59	−3.66
Permethrin	309	7.43	−6.29	−7.04	−7.44
Perthane	333	6.66	−7.04	−6.51	−6.75
Perylene	551	6.11	−8.80	−8.14	−8.83
p-Ethoxyacetanilide	407	1.67	−2.37	−2.26	−2.52
p-Ethyl hydroxybenzoate	389	2.49	−2.27	−2.90	−1.88
p-Ethylphenol	320	2.55	−1.40	−2.27	−1.46
p-Ethyltoluene	211	3.58	−3.21	−3.08	−3.12
p-Fluorobenzoic acid	458	2.07	−2.07	−3.17	−1.85
p-Fluorobenzyl chloride	298	2.99	−2.54	−2.49	−2.61
Phenacetin	408	1.67	−2.35	−2.27	−2.44
Phenallymal	431	1.68	−2.18	−2.51	−2.04
Phenanthrene	372	4.35	−5.19	−4.59	−5.11
Phenanthridine	380	3.32	−2.78	−3.64	−4.60
Phenetole	244	2.57	−2.33	−2.07	−2.30
Phenmedipham	416	3.27	−4.78	−3.95	−4.02
Phenobarbital	447	1.33	−2.32	−2.32	−1.95
Phenobenzuron	392	2.96	−4.32	−3.40	−6.00
Phenol	314	1.51	−0.06	−1.17	−0.36
Phenolphthalein	534	3.06	−5.20	−4.92	−5.94
Phenothrin	298	7.54	−5.24	−7.04	−6.97
Phenyl glycidyl ether	280	1.61	−1.80	−1.11	−1.30
Phenylacetic acid	350	1.43	−0.91	−1.45	−1.27
Phenylmethanol	258	1.08	−0.40	−0.58	−0.68
Phenytoin	568	2.16	−3.99	−4.36	−5.47
Phorate	298	3.37	−4.11	−2.87	−4.33
Phthalazine	365	1.12	−0.42	−1.28	−2.39
Phthalonitrile	412	1.09	−2.38	−1.73	−2.13
p-Hydroxyacetanilide	441	0.27	−1.03	−1.20	−0.49
p-Hydroxyacetophenone	382	1.19	−1.14	−1.53	−0.34
p-Hydroxybenzaldehyde	389	1.23	−1.16	−1.64	−0.85
p-Hydroxybenzyl alcohol	398	0.60	−1.27	−1.10	−0.22
p-Hydroxytoluene	308	2.06	−0.70	−1.66	−0.81
Picene	637	6.70	−7.81	−9.59	−10.68
Picric acid	394	1.54	−1.26	−2.00	−1.88
Pimilic acid	378	0.72	−0.51	−1.01	−0.44
Pindone	383	2.87	−4.11	−3.22	−1.96
Piperine	405	3.69	−3.46	−4.26	−2.91
Piperonal	311	1.77	−1.63	−1.40	0.14
Pirimicarb	364	1.40	−1.95	−1.56	−1.23
p-Isopropylbenzoic acid	391	3.33	−3.04	−3.76	−2.66
p-Methoxyacetanilide	400	1.18	−1.04	−1.70	−1.77
p-Methoxybenzaldehyde	275	1.79	−1.50	−1.29	−1.66
p-Methoxyphenol	329	1.59	−0.49	−1.40	−0.67
p-Methylacetophenone	301	2.22	−2.56	−1.75	−1.51
p-Methylbenzyl alcohol	333	1.62	−1.20	−1.47	−1.48
p-Nitroacetanilide	489	1.64	−1.91	−3.05	−2.45
p-Nitrobenzaldehyde	379	1.53	−1.81	−1.84	−2.29
p-Nitrobenzoic acid	512	1.69	−2.92	−3.33	−3.26
p-Nitrobenzyl alcohol	366	0.89	−1.88	−1.07	−1.44
p-Nitrophenol	388	1.91	−1.08	−2.31	−1.12
p-*N*-methylhydroxyaniline	360	0.79	−1.09	−0.91	−0.99
p-Phenylazoaniline	398	3.19	−3.79	−3.69	−4.13
p-Phenylenediamine	412	−0.39	−0.47	−0.25	−1.18
p-Propylphenol	294	3.04	−2.03	−2.54	−1.77
Prasterone	423	2.98	−3.66	−3.73	−3.92
Prasterone acetate	440	3.99	−4.46	−4.91	−4.98
Prednisolone	513	1.40	−3.21	−3.05	−2.78
Prednisolone acetate	505	2.14	−4.37	−3.71	−3.32
Prednisone	507	1.59	−3.48	−3.18	−1.99
Prednisonone-21-trimethylacetate	506	3.50	−4.58	−5.08	−4.75
Pregnenolone	466	3.89	−4.65	−5.07	−5.38
Primidone	554	0.73	−2.64	−2.79	−3.45
Prodiamine	397	4.94	−7.43	−5.43	−6.50
Profluralin	306	5.62	−6.54	−5.20	−5.30

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Progesterone	403	3.67	−4.55	−4.22	−5.09
Promecarb	360	3.18	−3.35	−3.30	−3.56
Prometon	365	3.57	−2.48	−3.74	−2.34
Prometryn	392	3.73	−3.86	−4.17	−3.64
Propachlor	345	2.42	−2.48	−2.39	−2.05
Propane	86	1.81	−2.85	−1.31	−1.45
Propanil	365	2.88	−3.22	−3.05	−2.94
Propazine	486	3.24	−4.43	−4.62	−4.65
Propene	88	1.68	−2.32	−1.18	−1.29
Propionanilide	379	1.59	−1.92	−1.90	−1.84
Propiophenone	292	2.16	−1.83	−1.66	−1.52
Propoxur	360	1.90	−2.05	−2.02	−2.67
Propyl 4-aminobenzoate	347	2.29	−2.33	−2.28	−2.51
Propyl 4-hydroxybenzoate	369	2.98	−2.56	−3.19	−2.32
Propyl acetate	180	1.36	−0.73	−0.86	−0.91
Propyl benzoate	222	2.81	−2.67	−2.31	−2.76
Propyl butyrate	178	2.34	−1.92	−1.84	−2.25
Propyl formate	180	0.81	−0.60	−0.31	−0.74
Propyl isopropyl ether	298	1.96	−1.34	−1.46	−2.06
Propyl propanoate	197	1.85	−1.34	−1.35	−1.43
Propyl propionate	197	1.85	−1.34	−1.35	−1.43
Propylcyclopentane	156	4.08	−4.74	−3.58	−3.14
Propyne	170	1.04	−0.41	−0.54	−0.79
Propyne	170	0.92	−1.04	−0.42	−0.79
Prostaglandin E2	340	3.52	−2.47	−3.44	−3.56
p-Terphenyl	486	5.52	−7.11	−6.90	−8.12
p-Toluic acid	453	2.42	−2.60	−3.47	−2.27
p-Toluidine	317	1.62	−1.22	−1.30	−1.55
p-Xylene	286	3.09	−2.82	−2.59	−2.61
Pyracarbolid	382	2.08	−2.56	−2.42	−2.65
Pyrazon	478	0.76	−2.87	−2.06	−2.16
Pyrazosulfuron-ethyl	455	0.25	−4.46	−1.32	−3.14
Pyrene	424	4.93	−6.18	−5.69	−5.79
Pyrrole	250	0.88	−0.17	−0.38	−0.42
Pyrrole	250	0.88	−0.17	−0.38	−0.42
Quinoline	258	2.14	−1.33	−1.64	−2.30
Quinone	389	0.25	−0.56	−0.66	−0.18
Quintozene	417	5.03	−5.82	−5.72	−5.97
Rimsulfuron	450	0.03	−4.63	−1.05	−2.54
Ronnel	308	4.86	−3.90	−4.46	−4.93
Rotenone	438	4.31	−4.42	−5.21	−5.75
S-(3,4-dihydro-4-oxobenzo[*d*]-[1,2,3]-triazin-3-ylmethyl) *O*,*O*-diethyl phoshorodithioate	322	3.51	−4.52	−3.25	−4.71
S-(3,4-dihydro-4-oxobenzo[*d*][1,2,3]-triazin-3-ylmethyl) *O*,*O*-dimethyl phoshorodithioate	345	2.53	−4.18	−2.50	−3.99
S-2,3,3-trichloroallyl diisopropylthiocarbamate	306	4.57	−4.88	−4.15	−4.62
Salbutamol	423	0.64	−1.22	−1.39	1.40
Salicin	471	−1.41	−0.85	0.18	0.62
Salicyl alcohol	357	0.60	−0.29	−0.69	0.16
Salicylaldehyde	266	2.01	−0.86	−1.51	−0.15
Santonin	444	1.78	−3.09	−2.74	−2.84
Sebacic acid	404	2.19	−2.31	−2.75	−2.87
Secbumeton	361	3.64	−2.56	−3.77	−2.86
sec-Butylbenzene	204	4.00	−3.76	−3.50	−3.52
Siduron	409	3.86	−4.11	−4.47	−4.14
Simazine	498	2.40	−4.51	−3.90	−4.40
Simetryn	356	2.90	−2.68	−2.98	−2.95
Styrene	242	2.89	−2.53	−2.39	−2.64
Styrene oxide	238	1.59	−1.60	−1.09	−1.42
Suberic acid	415	1.21	−1.17	−1.88	−1.37
Succinic acid	457	−0.75	−0.15	−0.34	0.15
Sulfabenzamide	454	1.30	−2.95	−2.36	−3.02
Sulfacetamide	456	−0.60	−1.23	−0.48	−1.16
Sulfacytine	440	−0.73	−2.23	−0.19	−1.97
Sulfadiazine	527	−0.34	−3.51	−1.45	−2.64
Sulfadimethoxine	475	1.17	−2.96	−2.44	−2.78
Sulfaethidole	459	0.90	−1.94	−2.01	−2.88
Sulfamerazine	509	0.21	−3.12	−1.82	−2.92
Sulfameter	488	−0.26	−2.58	−1.14	−2.59
Sulfamethazine	449	0.76	−2.27	−1.77	−2.76
Sulfamethizole	481	0.41	−2.41	−1.74	−2.40
Sulfamethomidine	419	0.75	−2.54	−1.46	−2.24
Sulfamethoxazole	440	0.48	−2.62	−1.40	−2.26
Sulfamethoxypyridazine	455	0.20	−3.28	−1.27	−2.64
Sulfamethylthiazole	512	1.26	−2.13	−2.90	−3.07
Sulfamoxole	467	1.03	−2.20	−2.22	−3.25

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Sulfaperine	535	0.21	−2.82	−2.08	−3.20
Sulfapyrazine	525	−0.34	−3.70	−1.43	−2.62
Sulfapyridine	463	0.53	−2.97	−1.68	−2.74
Sulfaquinoxaline	520	0.84	−4.60	−2.56	−4.00
Sulfathiazole	475	0.72	−2.84	−1.99	−2.20
Sulfathiozole	476	0.72	−2.43	−2.00	−2.21
Sulfisomidine	516	0.76	−2.24	−2.44	−3.48
Sulfisoxazole	467	1.03	−2.95	−2.22	−3.03
Sulfometuron-methyl	477	1.71	−3.17	−3.00	−3.70
Sulfosulfuron	475	0.99	−4.42	−2.25	−3.79
t-Amylbenzene	298	4.39	−4.15	−3.89	−3.80
Tebuthiuron	436	1.78	−1.96	−2.66	−2.09
Teflubenzuron	496	4.64	−7.30	−6.12	−6.91
Terbumeton	397	3.60	−3.24	−4.09	−3.07
Terbuthylazine	451	3.27	−4.43	−4.30	−4.22
Terbutryn	378	3.77	−3.98	−4.07	−3.80
Terbutryne	377	3.77	−4.00	−4.06	−5.19
tert-Amyl carbamate	358	1.34	−0.80	−1.44	−1.18
tert-Butyl bromide	256	2.54	−2.36	−2.04	−2.00
tert-Butyl chloride	248	2.45	−1.51	−1.95	−1.88
tert-Butylbenzene	215	3.90	−3.66	−3.40	−3.28
Testosterone	427	3.27	−4.09	−4.06	−4.38
Testosterone acetate	414	4.27	−5.18	−4.93	−4.81
Testosterone propionate	393	4.77	−5.37	−5.22	−5.24
Tetrabromomethane	363	2.80	−3.14	−2.95	−3.58
Tetrachloroethene	251	2.97	−2.91	−2.47	−3.09
Tetrachloroethylene	251	2.97	−2.74	−2.47	−3.09
Tetrachloroguaiacol	395	3.92	−4.02	−4.39	−3.81
Tetrachloromethane	250	2.44	−2.31	−1.94	−2.77
Tetradecane	279	7.22	−7.96	−6.72	−7.22
Tetrafluoroethylene	142	1.21	−2.80	−0.71	−1.26
Tetrafluoromethane	90	1.19	−3.68	−0.69	−2.25
Tetrahydropyran	228	1.43	−0.03	−0.93	−1.20
Tetramethysuccinic acid	464	0.99	−1.56	−2.15	−0.54
Theophylline	544	−0.39	−1.39	−1.57	−0.09
Thiazafluron	410	0.83	−2.06	−1.45	−1.53
Thioanisole	298	2.59	−2.39	−2.09	−2.39
Thiobencarb	276	3.90	−3.96	−3.40	−4.09
Thiofanox	330	2.16	−1.62	−1.98	−1.89
Thiophene	235	1.81	−1.45	−1.31	−0.98
Thymine	321	−0.32	−1.52	0.59	1.36
Thymol	324	3.52	−2.22	−3.28	−2.39
Tolbutamide	401	2.41	−3.39	−2.94	−3.84
Toluene	178	2.54	−2.24	−2.04	−2.13
Tranid	432	1.09	−2.08	−1.93	−1.76
trans-1,2-Dimethylcyclohexane	185	4.01	−4.33	−3.51	−3.37
trans-1,4-Dimethylcyclohexane	236	4.01	−4.47	−3.51	−3.37
trans-2-Butene	168	2.09	−2.04	−1.59	−1.46
trans-2-Heptene	164	3.91	−3.83	−3.41	−2.72
trans-2-Pentene	133	2.58	−2.54	−2.08	−1.97
trans-Azobenzene	341	4.11	−4.45	−4.04	−4.43
Triadimefon	355	2.94	−3.61	−3.01	−3.18
Triamcinolone	543	0.96	−3.69	−2.91	−2.50
Triamcinolone diacetate	508	1.51	−4.13	−3.11	−3.65
Triasulfuron	451	2.44	−4.10	−3.47	−3.58
Triazolam	497	3.96	−4.08	−5.45	−5.72
Tribromomethane	282	1.79	−1.91	−1.29	−2.14
Trichlorfon	356	−0.28	−0.22	0.20	−0.04
Trichlormethiazide	543	0.23	−2.68	−2.18	−3.10
Trichloroacetaldehyde	216	1.65	−0.69	−1.15	−0.51
Trichloroacetic acid	331	1.44	−0.57	−1.27	−0.25
Trichloroehylene	188	2.47	−1.96	−1.97	−2.43
Trichloroethylene	189	2.47	−2.01	−1.97	−2.43
Trichlorofluoromethane	162	2.43	−2.10	−1.93	−1.87
Trichloromethane	210	1.52	−1.18	−1.02	−1.78
Trichloronitromethane	209	2.09	−2.01	−1.59	−1.31
Tricyclazole	460	2.48	−2.07	−3.60	−3.24
Tridecanoic acid	315	5.49	−3.81	−5.16	−5.04
Trietazine	374	3.44	−4.06	−3.70	−3.87
Triflumuron	468	4.24	−7.16	−5.44	−6.48
Trifluoromethane	118	0.58	−1.23	−0.08	−1.39
Trifluoromethylbenzene	244	2.96	−2.51	−2.46	−1.49
Trifluralin	322	5.31	−6.26	−5.05	−6.17
Trimethoprim	474	0.73	−2.86	−1.99	−2.86

Appendix A (*Continued*)

Name	T_m (K)	ClogP	log S_w (M)		
			Exp	GSE	AQUAFAC
Trinitroglycerine	286	1.51	−2.22	−1.01	−2.12
Triphenylene	471	5.52	−6.74	−6.75	−7.55
Undecanedioic acid	385	2.68	−1.63	−3.05	−3.09
Undecanoic acid	302	4.51	−3.55	−4.04	−3.66
Valeraldehyde	182	1.31	−0.85	−0.81	−0.80
Veratrole	296	1.64	−1.31	−1.14	−1.89
Vernolate	298	3.51	−3.30	−3.01	−3.84
Vinyl acetate	181	0.73	−0.63	−0.23	−0.52
Vinyl chloride	119	1.62	−0.85	−1.12	−1.45
Warfarin	434	2.23	−3.89	−3.09	−4.10
XMC	372	2.27	−2.58	−2.51	−2.75
Xylylcarb	353	2.27	−2.49	−2.32	−2.52
Z-3-Chloro-2-butenoic acid	367	1.35	−0.61	−1.54	−0.75
α-Naphthol	369	2.69	−2.22	−2.90	−2.47
β-Naphthol	394	2.69	−2.28	−3.14	−2.50

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