PREDICTION OF AQUEOUS SOLUBILITY FROM SCRATCH

By

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PARIJAT JAIN

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DEDICATION

To my family

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ABSTRACT

Several methods have been proposed for the prediction of aqueous solubility. This study proposes the SCRATCH model for the aqueous solubility estimation of a compound directly from its structure. The algorithm utilizes predicted melting points and predicted aqueous activity coefficients for the solubility estimation, reflecting the truly predictive nature of the model. It uses two additive, constitutive molecular descriptors (enthalpy of melting and aqueous activity coefficient) and two non-additive molecular descriptors (symmetry and flexibility). The melting point prediction is trained on over 2200 compounds whereas the aqueous activity coefficient is trained on about 1640 compounds, making the model very rigorous and robust. The model is validated using a 10-fold cross- validation.

A comparison with the General Solubility Equation suggests that the SCRATCH predicted aqueous solubilities have a slightly more average absolute error. This could result due to the fact that SCRATCH uses two predicted parameters whereas the GSE utilizes only one predicted property. Although the GSE is simpler to use, the drawback of requiring an experimental melting point is overcome in SCRATCH which can predict the aqueous solubility of a compound just based on its structure and no experimental values.

CHAPTER 1

INTRODUCTION

Aqueous solubility is of fundamental importance for a variety of scientific and practical applications. It is a key factor in the successful development of new chemical drug entities. It directly affects the dissolution rate which, along with the permeability, influences the absorption rate and the bioavailablity of an orally administered drug.

Several techniques and methods are available for accurate solubility measurement. However, it can be difficult to measure solubility for very low solubility drugs. The advent of combinatorial chemistry and high throughput screening make it necessary to have reasonable means of estimating solubility from chemical structure alone, and to do it quickly and accurately.

The purpose of this research is to generate an algorithm to estimate the molar aqueous solubilities (S_w) for a wide range of organic compounds solely from their structures i.e., from scratch. The algorithm "SCRATCH" is designed to require no physical data as input (although experimental data will be used in generating a number of coefficients). Its development will lead to the ability to predict S_w early in the drug design process.

This proposal uses the aqueous activity coefficients (γ_w) which are calculated by group contribution (or q_i values) as well as two parameters related to the crystallinity of the solute, viz. melting point (T_m) and entropy of melting (ΔS_m). The calculated aqueous activity coefficients are based on experimental solubility values, whereas the entropy of

melting is calculated from two non-additive molecular descriptors, symmetry (σ) and flexibility (Φ).

The whole SCRATCH design falls under the realm of Yalkowsky's UPPER scheme (Yalkowsky et al., 1994). The UPPER stands for 'Unified Physicochemical Properties Estimation Relationships'. Figure 1 shows the flowchart of the inter-relationships of several physico-chemical properties that can be predicted using UPPER.

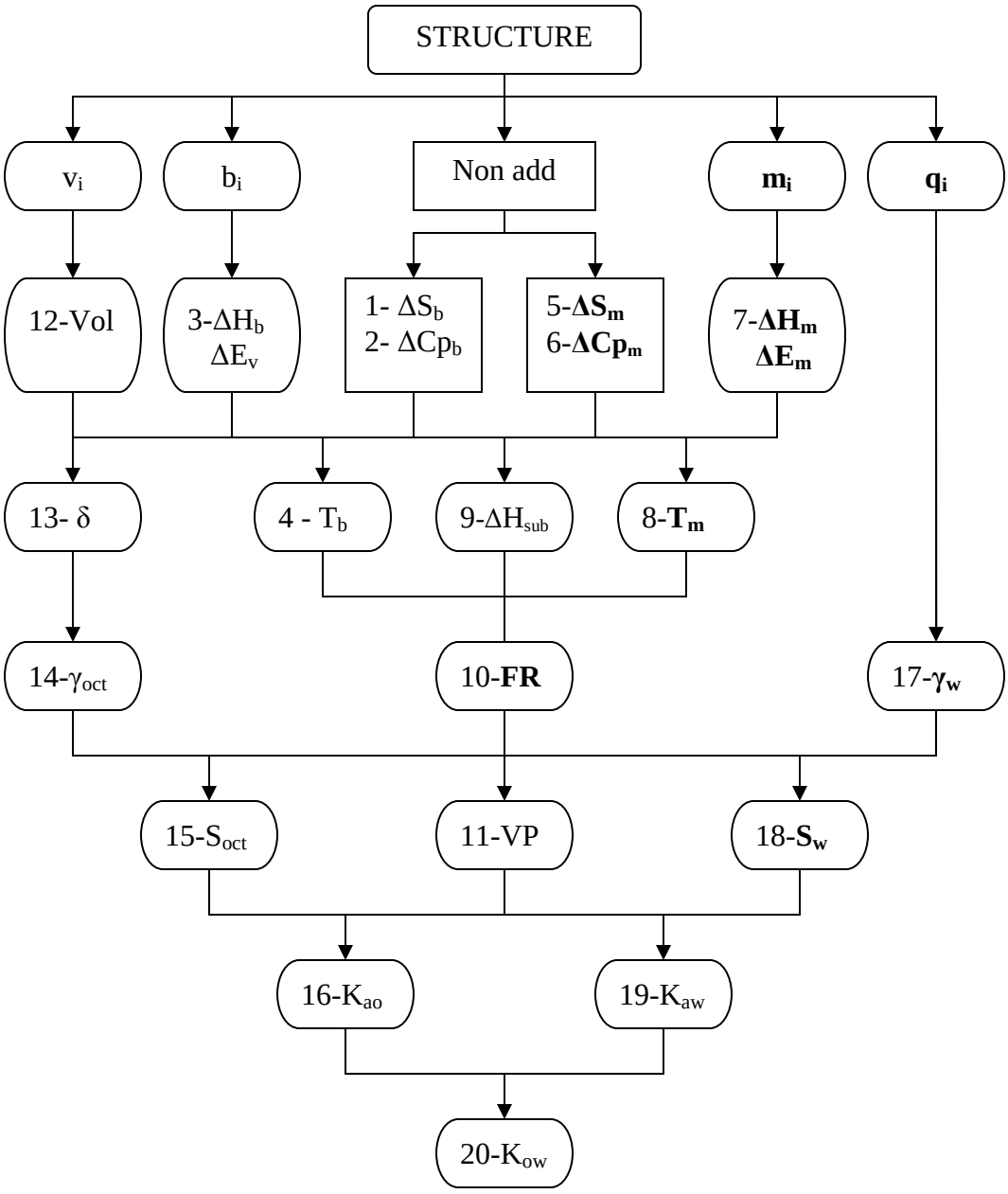

Figure 1.1. The UPPER Scheme

The properties incorporated in SCRATCH are indicated in bold in figure 1. Their symbols and abbreviations as well as their calculation will be discussed in the later chapters.

Chapter 2 deals with melting point estimation of a large dataset. The melting point is related to the enthalpy of melting (ΔH_m) and the entropy of melting (ΔS_m) by the following relationship.

$$T_m = \frac{\Delta H_m}{\Delta S_m} \tag{1.1}$$

The individual estimation of each of the above properties is discussed in detail. An alphabetical list of all the organic compounds studied, along with their σ and Φ values as well as their predicted and experimental melting points is reported in appendix A.

Chapter 3 discusses the calculation of aqueous activity coefficients using the AQUAFAC (AQUeous Functional Activity Coefficients) model, developed by Myrdal *et al.* This model utilizes a group contribution scheme, with coefficients that are based on experimental aqueous solubilities, to estimate the molar aqueous activity coefficients. A tabulation of molecular fragments and proximity factors along with their aqueous activity coefficient contribution values is provided. Appendix B lists the predicted and experimental activity coefficient values of organic compounds.

Chapter 4 shows the prediction of aqueous solubility from the SCRATCH algorithm. The coefficients obtained from chapters 2 and 3 for the melting points and the aqueous activity coefficients are used to calculate the aqueous solubilities. The prediction ability

of the SCRATCH is assessed using a 10-fold cross-validation. It is later compared with the General Solubility Equation (GSE) in terms of its applicability, usage and statistical fit. The experimental, the SCRATCH-predicted and the GSE-predicted aqueous solubility values are presented in appendix C.

Chapter 5 provides a final conclusion of the work.

A few of the equations may be repeated in the text of various chapters for a convenient explanation of the theory.

CHAPTER 2

ESTIMATION OF MELTING POINTS

2.1. Introduction

The melting point (T_m) is the transition temperature at which a substance changes from the solid state to the liquid state. It is one of the several properties that can be used to characterize a pure organic compound. Therefore, T_m is useful for compound identification and as a criterion for purity. It is used in the estimation of ideal crystalline solubility (X_i) which could further be used to calculate other important physicochemical properties such as vapor pressure (*VP*), octanol solubility (S_o) and aqueous solubility (S_w), as depicted in the UPPER scheme (figure 1).

Melting point data can be easily obtained at the early drug development stage. But it might be unavailable at the drug discovery phase when the drug is of low purity and is not crystallized. In the absence of experimental data, the melting point of a drug must be estimated from its structure. Several methods are available for predicting melting points from structure (Joback and Reid, 1987; Simmamora and Yalkowsky, 1994; Krzyzaniak et al., 1995; Austin, 1930; Constantinou and Gani, 1994; Marrero and Gani, 2001; Kier et al., 1976; Dearden et al., 1988; Abramowitz et al., 1990). Recently, Jain (2005) proposed a model to predict the melting points solely from the group contributions approach and two non additive constitutive geometric properties. We follow this model for the prediction of melting points for our dataset.

The Gibbs free energy of mixing, ΔG_{mix}, determines whether and to what extent two compounds mix to form a homogeneous phase (Yalkowsky, 1999). The free energy of mixing is defined as,

$$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix} \tag{2.1}$$

where, ΔH_{mix} is the enthalpy of mixing, ΔS_{mix} is the entropy of mixing and T is the temperature at which mixing occurs.

As mentioned earlier, melting is a solid to liquid transition. For a phase transition at equilibrium, the free energy change, ΔG_{mix}, is equal to zero. Therefore, equation (2.1) can be rearranged to obtain the equilibrium melting point,

$$T_m = \frac{\Delta H_m}{\Delta S_m} \tag{2.2}$$

.

2.1.1. Enthalpy of melting

The enthalpy of melting is the difference between the enthalpy of the solid and the liquid phases. It is defined as the heat required to melt one mole of a solid into liquid. It has been shown that the enthalpy of melting is an additive constitutive property (Jain, 2005). The heat of melting is dependent upon the interactions between the molecular fragments and is equal to the sum of its constituent group values (Krzyzaniak, 1995). It is given by,

$$\Delta H_m = \sum n_i m_i \tag{2.3}$$

where n_i is the number of times group i appears in the compound and m_i is the group contribution of group i to the heat of melting.

2.1.2. Entropy of melting

Entropy is the measure of randomness of molecules in a system. The total entropy of melting (ΔS_m^{tot}) includes entropies of all the solid-solid transitions and the solid-liquid transitions. Several approaches have been used for estimating the ΔS_m^{tot} of organic compounds. According to Bondi (1968), the total entropy of melting of a compound is the sum of its positional, rotational and conformational components:

$$\Delta S_m{}^{tot} = \Delta S_m{}^{pos} + \Delta S_m{}^{rot} + \Delta S_m{}^{conf} \tag{2.4}$$

Walden (1908) showed that the entropy of melting of aromatic, rigid, non-spherical compounds with little flexibility (coal tar derivatives) is constant at approximately 56.5 J/K-mol. Richard's rule states that the entropy of melting is constant for small spherical compounds (e.g., methane and neon) with a value of 10.5 J/K-mol. A large number of compounds do not belong to either of the above categories, and hence, cannot be reasonably estimated. Chickos et al. (1999) developed a group additive method for estimating the total entropy of melting. Although it has wide applicability, the method is cumbersome. Dannenfelser and Yalkowsky (1999) developed a semi empirical equation based on only two non-additive molecular descriptors, to estimate the total entropy of melting for nonelectrolytes,

$$\Delta S_m{}^{tot} = 50 - R\ln\sigma + R\ln\phi \tag{2.5}$$

where, R is the gas constant, 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:

$$\phi = 2.435^{\Phi} \tag{2.6}$$

where, $\Phi = SP3 + 0.5 \bullet (SP2 + RR) - 1$. The term *SP3* is defined as the number of nonring, nonterminal sp^3 atoms (such as CH_2, CH, C, NH, N, O, S etc.), *SP2* is the number of nonring, nonterminal sp^2 atoms (such as =CH, =C, =N etc.) and *RR* is the number of rigid single or fused ring systems. The expression for symmetry (σ) and flexibility (ϕ) can be substituted in equation (2.5) to obtain,

$$\Delta S_m^{\ tot} = 50 - 19.1 \bullet \log \sigma + 7.4 \bullet \Phi \tag{2.7}$$

It is important to realize that both molecular symmetry and flexibility are the properties of the whole molecule and are not group additive.

Recently, Jain et al. (2004) validated and applied equation (2.7) for a large data set of organic compounds.

2.2. Data

The dataset consist of a wide range of pharmaceutically and environmentally relevant organic compounds. The experimental melting points were collected from several electronic and print literature (Merck Index; Chemfinder website; AQUASOL® database; EPI Suite; Howard and Meylan, 1997; Chickos and Nichols, 2002; Jain and Yalkowsky, 2006).

2.3. Methods

Jain and Yalkowsky (2006) have published a list of molecular fragments and proximity factors along with their enthalpy contributions. These group coefficients are used to calculate the predicted enthalpy values using equation (3). The predicted entropy values are obtained using σ and Φ and equation 7. Finally, the melting points are estimated from the following equation, which is obtained by incorporating equations 2.3 and 2.7 into equation 2.2.

$$T_m = \frac{\Delta H_m}{\Delta S_m} = \frac{\sum n_i m_i}{50 - 19.1 \bullet \log \sigma + 7.4 \bullet \Phi} \tag{2.8}$$

The average absolute error (*AAE*) for each calculation was determined by

$$AAE = \frac{\sum \left| \log T_{m,\,pred} - \log T_{m,\exp} \right|}{N} \tag{2.9}$$

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

$$RMSE = \sqrt{\frac{\sum \left(\log T_{m,\,pred} - \log T_{m,\exp} \right)^2}{N}} \tag{2.10}$$

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

2.4. Results and Discussion

A complete alphabetical list of 883 organic compounds along with their σ *values*, Φ predicted melting points, experimental melting points, and calculation errors, is reported in appendix A. The compounds range from 85.5 K to 710.5 K in their melting points. Figure 2 shows the relationship between the experimental and the predicted melting points. The regression line has a slope of 0.989 and an R^2 of 0.841. The average

absolute error (AAE) in the prediction of melting points using Jain's (2005) model, for all the 883 compounds was observed to be 33.1 K whereas the RMSE was 43.3 K. The agreement in the predicted and experimental values can be seen from the near complete overlap of the trendline and the line of identity in figure 2.

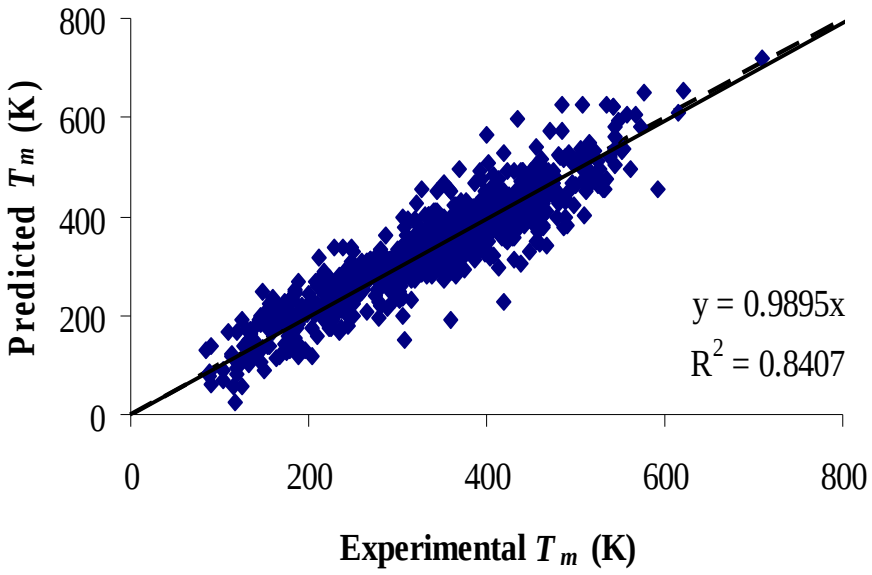

Figure 2.1. Plot of predicted and experimental melting points for 883 compounds. (solid line: regression line; dashed line: line of identity)

CHAPTER 3

ESTIMATION OF AQUEOUS ACTIVITY COEFFICIENTS

3.1. Introduction

Most solutions are not ideal solutions. This non-ideality may arise from a difference in either entropy of mixing or enthalpy of mixing. With water being the solvent, any hydrophobic solute would result in a highly non-ideal mixture owing to the difference between the water-solute interactions and the sum of the solute-solute and water-water enthalpic interactions. The addition of hydrogen bonding substituents to the organic compound would result in a lesser deviation from ideality. The extent of deviation from ideality is expressed by the activity coefficient, γ_w.

The behavior of a solute in solution is governed by its activity, *a*, which is defined as the ratio of its effective concentration (fugacity or escaping tendency) in the solvent compared to that in the pure liquid state. The mole fractional activity coefficient, γ_w, of a solute relates activity to its mole fractional concentration, x_w, by

$$\gamma_w = \frac{a_w}{x_w} \tag{3.1}$$

where the subscript *w* represents the water phase. Since, the deviation from ideal solubility is described by the aqueous activity coefficient, γ_w, the activity of the solute must be equal in both phases when a liquid solute is in equilibrium with water. Therefore,

$$x_w \bullet \gamma_w = x_o \bullet \gamma_o \tag{3.2}$$

where the subscript *o* refers to the organic phase. For liquids that are poor solvents for water, the organic phase is essentially the pure liquid solute, and x_o and γ_o can both be approximated by unity. In other words the activity of an infinitely dilute solute is equal to unity. Thus,

$$x_w = \frac{1}{\gamma_w} \tag{3.3}$$

and,

$$\log x_w = -\log \gamma_w \tag{3.4}$$

Hence, for hydrophobic compounds, techniques for estimating γ_w are essentially equivalent to those for estimating x_w.

The AQUAFAC (AQqueous Functional Activity Coefficient) model, of Myrdal *et al.*, utilizes a group contribution scheme based on experimental aqueous solubility data to estimate molar aqueous activity coefficients (Myrdal *et al*., 1992, 1993, 1995; Pinsuwan et al., 1997). According to this model, the aqueous activity coefficient of a compound is determined using the summation of simple additive constitutive group values, i.e.

$$\log \gamma_w = \sum n_i q_i \tag{3.5}$$

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. It is important to note that the same molecular fragmentation scheme is used for calculating both enthalpies of melting and aqueous activity coefficients

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

$$S_w = \frac{X_i^c}{\gamma_w} \bullet 55.5 \tag{3.6}$$

where, X_i^c is the ideal crystalline mole fraction solubility and 55.5 mol/L is the molarity of water.

Equation (3.6) can be combined with the Van't Hoff equation (discussed in Chapter 4) to give,

$$\log \gamma_w = 1.74 - \log S_w - \frac{\Delta S_m (T_m - T)}{2.303 \bullet R \bullet T} \tag{3.7}$$

where ΔS_m is the entropy of melting and T_m is the melting point. Chapter 4 discusses the derivation of equation (3.7) in detail.

3.2. Molecular fragmentation

Hansch and Leo (1979) introduced the concept of an 'isolating carbon'. It is defined as the carbon that is not doubly or triply bonded to a hetero-atom. Each molecular fragment then is the smallest group of atoms (consisting of all carbons, hydrogen, and hetero atoms, including their non-bonded electrons) that are not separated by an isolating carbon. This helps in the breakdown of any organic structure into fragments varying from single atoms like C, N, Br to large polyatomic groups like >SO2NHC(=O)NH- of the sulfonylureas and C(=O)NHC(=O)NHC(=O)- of the barbiturates. (Note that the entire barbiturate ring can be defined as an alternate single fragment if desired.) Leo (1993) applied this breakdown scheme successfully in the fragmentation scheme of ClogP. Over the years the concept has been elaborated and

several chemical groups have been added. Jain and Yalkowsky (2006) have published the latest modification. This study uses the same scheme for the breakdown of the compounds.

3.3. Data

The experimental molar aqueous solubilities of 1642 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. The experimental melting points were collected from the sources mentioned in Chapter 2. 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.

3.4. Methods

All the compounds are fragmented into 147 groups using a modification of the breakdown scheme of Jain and Yalkowsky (2006). The data set containing the aqueous activity coefficients and group counts was prepared in Microsoft Excel 2000. Multiple linear regression against the experimental activity coefficients was performed using SPSS for Windows version 10.0 (SPSS Inc., Chicago, IL). The regression analysis generated the group contribution values, q_i, which, when substituted in equation (3.5), provided the predicted aqueous activity coefficients. Equation (2.5) has been used to calculate the predicted entropies of melting using the symmetry (σ) and the flexibility

(ϕ) numbers. The average absolute error (AAE) and the root mean square error (RMSE) were calculated as explained in Chapter 1.

3.5. Results and Discussion

Appendix B contains an alphabetical list of all the compounds along with their predicted and experimental activity coefficients. Table 3.1 provides the coefficients of the 147 groups into which the compounds were broken down. These coefficients form the basis for activity coefficient estimation of new compounds. Table 3.2 defines the various group environments and the proximity factors used in table 3.1.

Table 3.1. A list of molecular fragments and proximity factors along with their aqueous activity coefficient contribution values

Groups	All	YY	Y	X	ar	br	bp	ring	fus
>C<		-1.18	-1.81	-1.51	0.00	0.15	-0.15	-0.72	-0.69
>C=		-1.68	-0.35	-0.16				0.15	-0.80
-C#				0.39					
>CH		-1.28	-0.75	-0.60	0.57			-0.05	-0.13
-CH=								0.65	
-CH#	1.09								
>CH2		0.24	0.23	0.53				0.63	
=CH2	1.43		0.12	0.55					
-CH3			1.05	1.33					
-CH(=O)			0.45	-0.07					
-CN			0.37	0.51					
>CN=	-1.95								
-C(=O)N<			-2.44	-3.05				-0.52	
-C(=O)NH-			-2.34	-1.73				-0.99	
-C(=O)NH2			-0.52	-0.77					
-C(=O)N(S-)C(=O)-	-0.19								
-C(=O)NHC(=O)N HC(=O)-	-1.96								
>C(=O)		-1.02	-1.13	-0.56	0.19			-0.66	
-C(=O)O-			-0.70	-0.78	0.22			-0.98	
CH(=O)O-	0.10								
-C(=O)OH			-0.65	-0.43					
-F			0.74	1.00					
-Cl			1.20	1.14					
-Br			1.47	1.25					
-I			1.82	1.69					
>N-			-1.62	-2.48	-0.22	0.12		-2.13	
>NH		-1.07	-0.62	-3.89	-0.10			-1.11	
-NH2			-0.20	-0.69					
-N=N-	0.02								
-NC(=O)N-								-1.35	
-NC(=O)NH-	-3.05								
-N1C(=O)NC(=O)O1	-0.43								
-NH(Cl-triazine)N<	-0.97								
-NH(Cl-triazine)NH-	-0.23								
-NH(O-triazine)NH-	-2.18								

Table 3.1. Continued..

Groups	All	YY	Y	X	ar	br	bp	ring	fus
-NH(S-triazine)NH-	-1.21								
-NHC(=O)ON=C<	-2.14								
-NHC(=O)ON=CH-	-1.30								
-NHC(=O)ON=C(-)S-	-2.17								
-NHCONH-	-2.42								
-NHCONH2	-1.80								
-NHCONHCO-	-1.44								
-NHCONO-	-2.48								
-NHCSNH-	-0.79								
-NHNO2	0.38								
-NN-					0.01				
-NN(-)C(=O)-	-1.89								
-NNN(-)C(=O)-	-0.22								
-NO-	0.20								
-NO2			0.69	0.73					
>N(NO2)	0.18								
=NHC(=O)N-C(=O)-	-2.01								
>NC(=O)N-C(=O)-	-3.03								
>O		0.78*	-0.65	-1.37	0.64			-0.23	
-OH			-0.83	-0.64					
-OC(=O)NH2	-0.82								
OCH(=O)								0.16	
-OC(=O)N<	-3.20								
-OC(=O)NH-	-1.47								
-ONO2	1.14								
P(O-)2(=S)(S-)	-0.25								
-P(=O)(O-)2	-2.89								
P(O-)3(=S)	-0.83								
-P(=S)(O-)2	-1.40								
P(=S)(O-)2(S-)	-0.47								
P(=S)(O-)3	-0.36								
-S-			-0.03	0.23	0.46			1.09	
-SC(=O)N<	-1.57								
-SH				0.93					
>S(=O)	-2.08								

*The group is a YY Oxygen in an aliphatic ring

Table 3.1. Continued..

Groups	All	YY	Y	X	ar	br	bp	ring	fus
>SO2			-0.59	-0.77				0.10	
-SO2NH-	-1.38								
-SO2NH2	-0.52								
-SO2NHCH=N-	-1.40								
-SO2NHCO-	-1.90								
-SO2NHCONH-	-2.26								
Proximity factors									
IHB5	-0.18								
IHB6	0.27								
IHB7	0.48								
2 OH	-0.56								
3 OH	-0.59								
G2	0.16								
G3	0.72								
G4	1.48								

Table 3.2. Description of various group environments and proximity factors

Symbol	Description
X	The fragment is attached to singly bonded group
Y	The fragment is attached to a doubly or triply bonded group
YY	The fragment is attached to two or more doubly bonded groups
ar	The fragment is attached to an aromatic ring
br	The carbon atoms acting as a bridge between two aromatic rings
bp	The central carbons that are a part of two phenyl rings, hence known as biphenyl
Ring	An aliphatic ring system
2°, 3°	Secondary and tertiary aliphatic, respectively
IHB -5, -6, -7	Possible intra hydrogen bonding producing 5, 6, or 7 member ring systems
G -2, -3, -4	Carbons bound to two, three or four halogens, respectively

Figure 3.1 shows the relationship between the experimental and the predicted aqueous activity coefficients. The regression line has a slope of 0.983 and an R^2 of 0.898. The average absolute error (AAE) in the prediction of aqueous activity coefficients for all

the compounds is 0.465 log units and the RMSE is 0.653. It is important to realize that the training set and the test set are the same. Therefore the errors are based upon 'fit' rather than prediction. Over 88 % of the activity coefficients are estimated within one log unit of their observed values. This is reflected in the overlap of the trendline and the line of identity in figure 3.1.

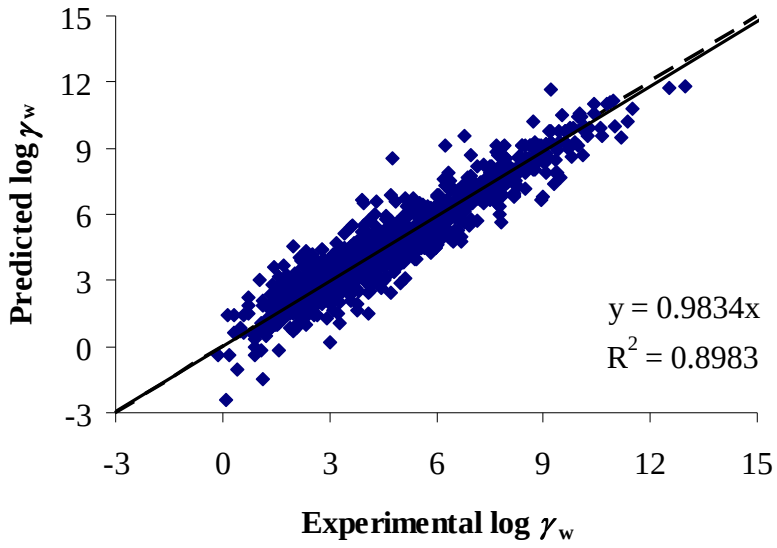

Figure 3.1. Plot of predicted and experimental aqueous activity coefficients (γ_w) for 1642 compounds. (solid line: regression line; dashed line: line of identity)

CHAPTER 4

PREDICTION OF AQUEOUS SOLUBILITY FROM SCRATCH

4.1. Introduction

Aqueous solubility is the equilibrium concentration of a substance in water. It is one the most important physico-chemical factors that affect the dissolution, the absorption and in turn the bioavailability of the drug. Poor aqueous solubility is a common problem that frequently poses a challenge in the formulation development stage. Present work aims to predict the aqueous solubility of a compound solely by its chemical structure.

Several methods are available for aqueous solubility prediction. The GSE (General Solubility Equation) and the AQUAFAC (AQUeous Functional group Activity Coefficients) are two such empirical models for aqueous solubility prediction. Both these methods require experimental melting point data, which could be a limitation at the early drug discovery phase. The proposed model predicts the aqueous solubility without the use of any experimental melting point data. The method uses the predicted activity coefficients from the AQUAFAC model of Chapter 3) and the predicted melting points obtained from the group contribution approach of Chapter 2. Thus, the aqueous solubilities obtained from our model are true prediction values.

4.2. Aqueous Solubility for liquid solutes

The techniques for estimating the mole fraction concentration of a hydrophobic compound are essentially equivalent to those for estimating the aqueous activity coefficients (γ_w). As mentioned previously (chapter 3),

$$x_w = \frac{1}{\gamma_w} \tag{4.1}$$

and

$$\log x_w = -\log \gamma_w \tag{4.2}$$

The aqueous activity coefficient is a group additive constitutive property and can be obtained from Myrdal et al.'s AQUAFAC model, using the following relationship,

$$\log \gamma_w = \sum n_i q_i \tag{4.3}$$

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.

The molar solubility of a liquid in water is

$$S_w^{\ l} = \frac{1}{\gamma_w \cdot v_w} \tag{4.4}$$

where, v_w is the molar volume of water, 0.0182 L/mol.

4.3. Aqueous solubility for solid solutes

In the case of solids, it is necessary to account for the impeding effect of crystallinity upon solubility. The solubility of a crystalline solute in any solvent is equal to the product of its crystal:liquid solubility ratio and the reciprocal of its activity coefficient at infinite dilution in that solvent. Thus, for a crystalline solute in water, the molar aqueous solubility (S_w) for poorly soluble solutes, is given by

$$S_w = \frac{(x^c / x^{scl})}{\gamma_w \cdot v_w} \tag{4.5}$$

where, x^c/x^{scl} is the ratio of the solubility of the crystal to that of the hypothetical super cooled liquid. The above equation may be written as,

$$S_w = \frac{X_i^c}{\gamma_w} \bullet 55.5 \tag{4.6}$$

where X_i^c is the ideal crystalline mole fractional solubility and 55.5 mol/L is the molarity of water. Taking logarithms on both sides of equation (4.6) gives,

$$\log X_w = \log X_i^c - \log \gamma_w - 1.74 \tag{4.7}$$

It is well known that the solubility of a crystalline solute in any solvent is dependent upon the properties of the crystal. The solubility reduction that is attributable to crystallinity is given by the van't Hoff equation

$$\log X_i^c = -\frac{\Delta H_m (T_m - T)}{2.303 \bullet R \bullet T_m \bullet T} + \frac{\Delta C_p}{2.303 \bullet R}\left(\frac{T_m - T}{T} - \log \frac{T_m}{T}\right) \tag{4.8}$$

or,
$$\log X_i^c = -\frac{\Delta S_m (T_m - T)}{2.303 \bullet R \bullet T} + \frac{\Delta C_p}{2.303 \bullet R}\left(\frac{T_m - T}{T} - \log \frac{T_m}{T}\right) \tag{4.9}$$

where, ΔH_m, ΔS_m and ΔC_p are the enthalpy, entropy and the heat capacity differences between the solid and the liquid forms of the material respectively, T_m is the melting point and T is the temperature of interest (both in Kelvin).

The above equation can be simplified on the basis of one or both of the following assumptions: (1) that the value of ΔC_p is close to zero and (2) that the two terms in parenthesis are nearly equal for most organic compounds at 300 K. Mishra and Yalkowsky (1990) verified the applicability of the first assumption for a wide variety of organic compounds. Eliminating the heat capacity term enables approximating equation (4.8) by

$$\log X_i^c = -\frac{\Delta H_m (T_m - T)}{2.303 \bullet R \bullet T_m \bullet T} \tag{4.10}$$

Thus, the molar aqueous solubility (S_w) of solid solutes in water at room temperature can be given by substituting equation (4.10) into equation (4.7), to give,

$$\log S_w = 1.74 - \log \gamma_w - \frac{\Delta H_m \bullet (T_m - 298)}{2.303 \bullet 298 \bullet R \bullet T_m} \tag{4.11}$$

$$\log S_w = 1.74 - \log \gamma_w - \frac{\Delta S_m \bullet (T_m - 298)}{2.303 \bullet 298 \bullet R} \tag{4.12}$$

$$\log S_w = 1.74 - \log \gamma_w - \frac{\Delta S_m \bullet (MP - 25)}{2.303 \bullet 298 \bullet R} \tag{4.13}$$

Assuming the Walden's rule for entropy of melting (ΔS_m) (being equal to 56.7 J/mol-K), the above equation may be written as,

$$\log S_w = 1.74 - \log \gamma_w - 0.01(MP - 25) \tag{4.14}$$

where *MP* is the melting point of the solute in Celcius

4.4. General Solubility Equation (GSE)

The GSE (Jain and Yalkowsky, 2001; Ran *et al.*, 2001) is based on the fact that the aqueous solubility of a solute depends upon its crystallinity as described by equation 4.14 and its polarity, which is a measure of its octanol-water partition coefficient ($\log K_{ow}$), using the following expression:

$$\log S_w = 0.5 - 0.01(MP - 25) - \log K_{ow} \tag{4.15}$$

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. This is applicable to most uncharged organic molecules.

3. The heat capacity of melting (C_{pm}) 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.

4.5. Methods

The molar aqueous solubility (S_w) of an organic compound can be obtained from its activity coefficient (γ_w), enthalpy of melting (ΔH_m) and melting point (T_m) values using equation (4.11).

The enthalpy of melting is calculated by $\Delta H_m = \sum n_i m_i$, where the m_i values are the group contributions to the heat of melting. As illustrated in chapter 2, the melting points for 883 organic compounds were predicted from the Jain's (2005) model, using the ΔH_m and the ΔS_m. The latter is calculated by,

$$\Delta S_m^{\ tot} = 50 - 19.1 \bullet \log \sigma + 7.4 \bullet \Phi \qquad (4.16)$$

where the rotational symmetry number (σ) and the flexibility number (Φ), are the non-additive molecular parameters. This gives the following equation,

$$T_m = \frac{\Delta H_m}{\Delta S_m} = \frac{\sum n_i m_i}{50 - 19.1 \bullet \log \sigma + 7.4 \bullet \Phi} \tag{4.17}$$

The data for the aqueous activity coefficients for the same organic compounds were obtained using the Jain et al. (2007) model, which uses the sum of group contribution values of the compounds for the activity coefficients ($\sum n_i q_i$), as previously described in chapter 3.

Finally, equations (4.14) and (4.17) are combined to give the following relationship for the prediction of solubility at 298 K,

$$\log S_w = 1.74 - \log \sum (n_i q_i) - \frac{\sum n_i m_i - 298 \bullet (50 - 19.1 \bullet \log \sigma + 7.4 \bullet \Phi)}{5709} \tag{4.18}$$

This solubility is termed the solubility predicted from scratch since only the chemical structure of the solute is needed. The SCRATCH solubility is compared with the GSE-predicted solubility for the same set of compounds.

4.6. Experimental

The partition coefficients (logK_{ow}) for the GSE were obtained from EPI Suite. The average absolute errors (AAE) and the root mean square errors (RMSE) were calculated as explained in Chapter 1.

The experimental melting points as well as solubilities were collected from WATERNT™ v 1.0 EPA and AQUASOL databases. Each compound was broken down

into groups using Jain and Yalkowsky's (2005) scheme and the m_i and q_i were determined by regression using SPSS software.

A ten-fold cross-validation experiment was performed on the complete data set. For each validation, approximately $1/10^{th}$ of the data were randomly selected using the RAND function in Microsoft Excel 2000, and used as a test-set. Each compound was included only once in the 9 training sets or in a test set. Each round was run in the following manner: The test-set compounds were deleted from the complete enthalpy data (2230 compounds) and from the aqueous activity coefficient data (1642 compounds). The remaining compounds in both data sets were treated as the training sets. Any compound in the test set with a group or fragment not present in the training set was deleted from the test set. This was done to ensure true prediction from the training set. Regressions were run to obtain the enthalpic– as well as the activity coefficient–group contribution values, m_i and q_i, respectively. These were then used to obtain the solubility values for the test-set.

In order to better understand the source of errors, the aqueous solubility was calculated using various combinations of crystal term (predicted or experimental) and the liquid term or the activity coefficient (partition coefficient or sum of group contributions).

4.7. Results and Discussion

The complete alphabetical list of 883 organic compounds along with their melting points, partition coefficients, experimental as well as their SCRATCH and GSE-predicted aqueous molar solubilities is provided in appendix C.

A plot of experimental versus the predicted aqueous activity coefficients for this dataset yields a regression line with a slope of 0.976 and an R^2 of 0.859 (figure 4.1). The average absolute error (AAE) in the prediction of aqueous activity coefficients is 0.484 log units and the RMSE is 0.674.

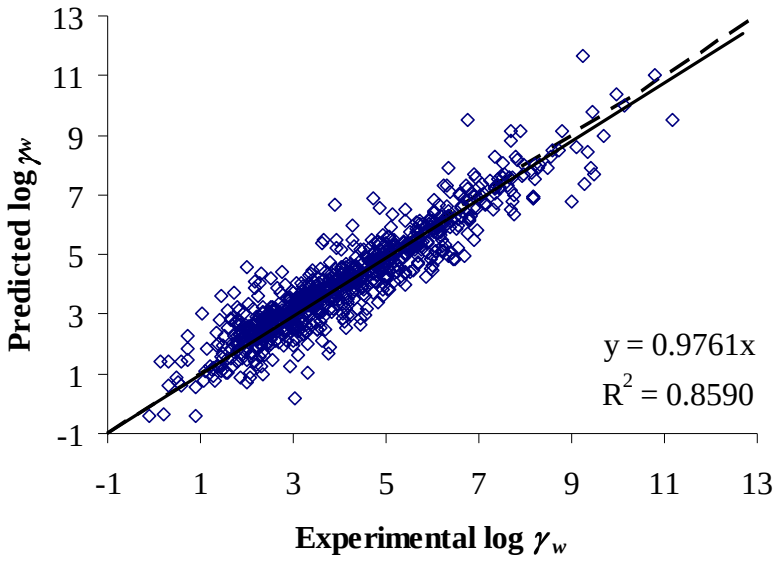

Figure 4.1. Plot of predicted and experimental aqueous activity coefficients (γ_w) for 883 compounds. (solid line: regression line; dashed line: line of identity)

Figure 4.2 shows the relationship between the experimental and the SCRATCH–predicted aqueous solubilities. The regression line has a slope of 0.956 and an R^2 of 0.859. The AAE in the prediction of aqueous solubilities for all the compounds is 0.535 log units while the RMSE is 0.719. About 84 % of the molar solubilities were predicted within one log unit of their observed values. These results are noteworthy considering the size and diversity of the compounds which span over 10 orders of magnitude in terms of molar aqueous solubility. The solubilities obtained using SCRATCH, are purely predicted with no experimental data required. This is a major advantage over other existing models.

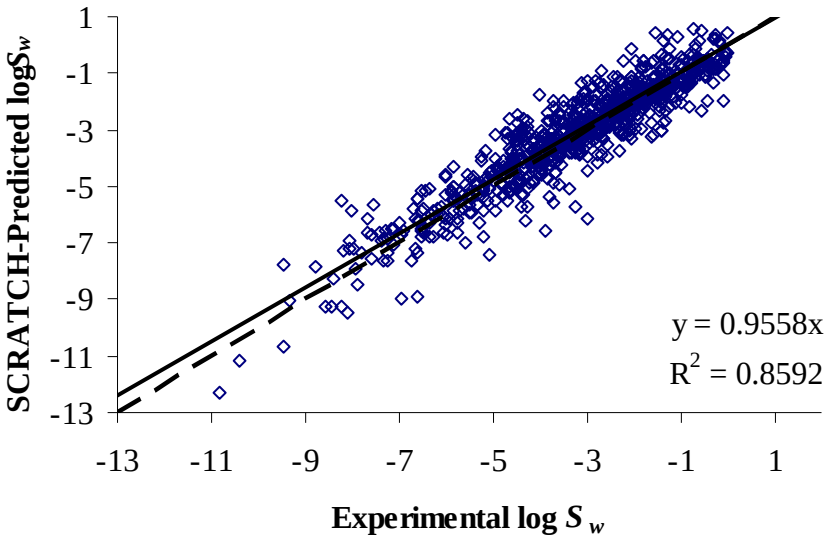

Figure 4.2. Plot of logarithm of experimental and SCRATCH-predicted aqueous molar solubilities. (solid line: regression line; dashed line: line of identity)

4.7.1. Comparison with the GSE

The General Solubility Equation is a widely used method to calculate solubility. In this section, the GSE is applied to the same set of compounds and the prediction results are

compared with our model. Table 4.1 summarizes the results of the SCRATCH and GSE-estimated solubilities. A plot of the experimental versus the GSE-predicted aqueous solubilities (figure 4.3) resulted in a slope of 0.912, an R^2 of 0.781 and an AAE of 0.656 log units (table 4.1). About 77.6% of the GSE molar aqueous solubilities are predicted within one log unit of their observed values. The regression line is much closer to the line of identity in figure 4.2 than in figure 4.3, indicating that the estimates from the SCRATCH model are closer to the true values than the estimates from the GSE.

Table 4.1. Results of aqueous solubility estimations

	SCRATCH-pred	**GSE-pred**
Number of compounds	883	883
Slope	0.956	0.912
R^2	0.859	0.781
AAE (log unit)	0.535	0.656
RMSE (log unit)	0.719	0.863
Error ≤ 1 log unit	83.80 %	77.60 %

The major assumption in the GSE is that 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.

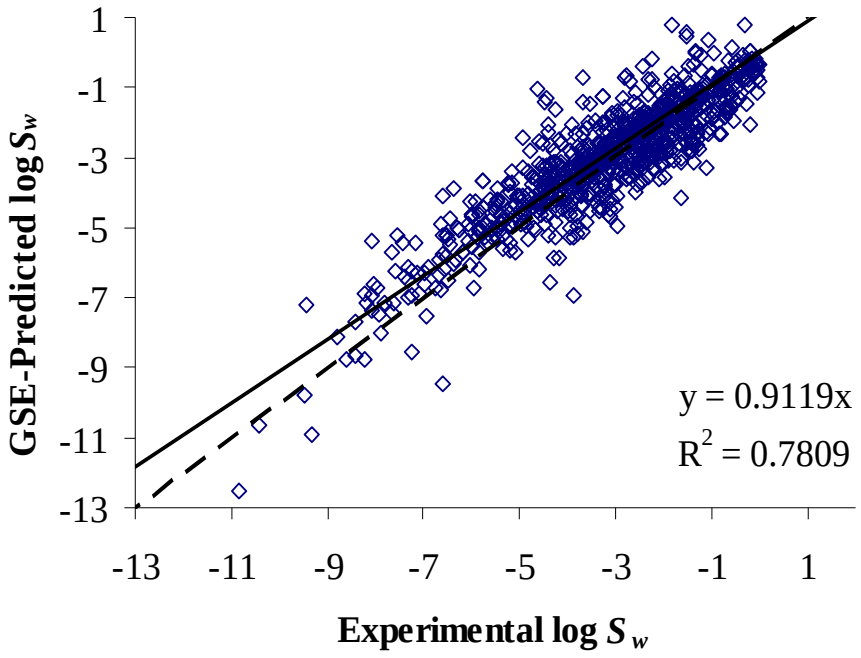

Figure 4.3. Plot of logarithm of experimental and GSE-predicted aqueous molar solubilities for 883 compounds. (solid line: regression line; dashed line: line of identity)

The GSE utilizes the experimentally determined melting points and ClogP values (which are based upon group contributions) while the SCRATCH equation utilizes two sets of group contribution values, m_i, and q_i. The first along with entropic factors (σ and Φ) gives a reasonable estimate of the role of crystallinity in determining solubility. The latter is based upon experimental aqueous solubility data.

The crystal term is more accurate in the GSE because the actual melting point is used. On the other hand the activity coefficient is more accurate with the SCRATCH equation

because it is based directly on solubility data whereas the GSE utilized ClogP to estimate the activity coefficient.

Overall, the GSE is simpler but the SCRATCH equation is slightly more accurate. Also, the GSE requires an experimental value whereas the SCRATCH does not.

4.7.2. Cross-validation

The results of the cross-validation are shown in table 4.2. The AAE of the aqueous solubilities in logarithmic units of each test set are given in the last column. The overall mean AAE of the ten rounds is 0.760. This value is the true prediction error of the SCRATCH model. The AAE of 0.535 obtained in section 4.7 is a result of fitting since the test set is included in the training set. Therefore, the absolute errors of GSE (0.656) and SCRATCH (0.760) are based on true predictions. In this sense the GSE performs slightly better (~0.1 log unit or a factor of 1.26) than the SCRATCH.

Table 4.2. Ten-fold cross-validation of the SCRATCH model

	Training set			Test set	
	Melting point	**Activity Coefficient**	**Size**	**Deleted**	**AAE**
Round 1	2142	1553	87	1	0.771
Round 2	2142	1553	88	0	0.774
Round 3	2142	1553	86	2	0.941
Round 4	2142	1553	85	3	0.730
Round 5	2142	1553	88	0	0.755
Round 6	2142	1553	86	2	0.877
Round 7	2142	1553	88	0	0.649
Round 8	2142	1553	88	0	0.634
Round 9	2142	1553	88	0	0.813
Round 10	2142	1553	91	0	0.658
Average					0.760
Complete			883		0.535

4.7.3. Sources of error in solubility prediction

The crystalline contribution to the solubility is given by the ideal crystalline term which is mainly determined by the melting point (T_m) and the calculated activity coefficient ($\log K_{ow}$ or $\sum n_i q_i$) represents the liquid contribution to the aqueous solubility. Various

combinations of experimental and predicted melting points and activity coefficients lead to different models. Table 4.3 shows the SCRATCH and the GSE models and the AAE in the determination of the aqueous solubilities of 883 compounds using those models.

Table 4.3. Sources of error in determining aqueous solubility (n=883)

Model	Crystal term (Ideal solubility)	Liquid term (Activity Coefficient)	Overall (log units)
	T_m	γ_w	
GSE	Exp	LogP	0.66
SCRATCH	$\sum n_i m_i / \Delta S_m$	$\sum n_i q_i$	0.76*

Exp: experimental
*: values obtained from 10-fold cross validation

The GSE uses experimental T_m and the calculated partition coefficient for solubility estimation whereas in SCRATCH both the terms are calculated. The propagation of errors associated with the prediction of two terms in SCRATCH, could lead to a higher AAE than the GSE. This is indeed true, as seen in table 4.3. The AAE of 0.76 from the crystal term in the SCRATCH comes from the error in melting point (33.1 K, section 2.4) as well as from the predicted activity coefficients (0.46, section 3.4) .

Although GSE is better than SCRATCH in terms of the AAE, it is worth noting that both the models differ only by 0.1 log units. This provides a great flexibility to the user in terms of using any of the above models depending on the type of data available.

CHAPTER 5

CONCLUSION

The SCRATCH is a semi-empirical algorithm for the estimation of aqueous solubilities using predicted melting points and aqueous activity coefficients.

The average absolute error in the prediction of melting points using Jain and Yalkowsky's (2005) model for a test set of 883 compounds is observed to be 33.1 K. A good agreement (R^2 = 0.841) exists between the predicted and experimental melting points.

Over 88% of the activity coefficients of 1642 organic compounds are predicted within one log unit of their observed values. The average absolute error in the prediction of aqueous activity coefficients for all the compounds is 0.465 log units.

The melting points and the activity coefficients are finally used to obtain the aqueous solubilities of 883 compounds using SCRATCH. A comparison shows that the GSE is slightly more accurate than the SCRATCH model for the compounds tested. This could be explained by the fact that the SCRATCH uses predicted melting points and predicted aqueous activity coefficients. Since the errors from both the predicted values can propagate, the average error can be expected to be greater than that of the GSE in which only one property (the partition coefficient) is predicted.

The GSE requires experimental melting points for the solubility prediction whereas the SCRATCH does not need any experimental value which is a big advantage in the early drug discovery phase for newly synthesized compounds, when the drug is not completely characterized or the experimental melting points are not available. The model is cross-validated to confirm its prediction ability.

The 147 groups into which the compounds are broken down account for the wide range of structural variation. The developed model provides an accurate and widely applicable tool for estimation of aqueous solubility values of organic compounds from their chemical structures, two sets of group contribution values and two non-additive geometric parameters.

APPENDIX A. Experimental and Predicted enthalpy of melting (ΔH_m) and melting points (T_m) along with the molecular symmetry number (σ) and molecular flexibility number (Φ) for 883 compounds.

	ΔH_m (KJ/mol)		σ	Φ	T_m (K)	
Name	**Exp**	**Pred**			**Exp**	**Pred**
(+)a-(3-benzoylphenyl)propionic acid	28.2	23.5	1	1.0	367.4	409.1
(2,4,5-trichlorophenoxy)acetic acid	38.0	26.7	1	2.0	431.2	412.6
(2,4-dichlorophenoxy)acetic acid	35.3	26.7	1	2.0	412.5	412.6
(4-chloro-2-methylphenoxy)acetic acid	30.0	25.5	1	2.0	392.9	393.1
(4-chloro-o-tolyloxy)acetic acid	30.0	25.5	1	2.0	392.9	393.1
(d) 1,2-diphenyl-1,2-dihydroxyethane	34.3	25.8	1	2.0	420.5	398.8
(d) 2-(m-chlorophenoxy)propanoic acid	29.7	25.0	1	2.0	367.5	386.0
(d) methylenebisthiopropionic acid	22.6	33.3	1	5.0	355.0	382.7
(dl) 1,2-diphenyl-1,2-dihydroxyethane	31.4	25.8	1	2.0	393.0	398.8
(dl) 2-(m-chlorophenoxy)propanoic acid	33.1	25.0	1	2.0	386.0	386.0
(dl) menthol	10.3	16.7	1	3.0	301.2	231.6
(dl) methylenebisthiopropionic acid	39.3	33.3	1	5.0	429.0	382.7
(l) menthol	11.9	16.7	1	3.0	316.2	231.6
1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	22.9	28.8	1	3.0	351.4	399.4
1-(methylamino)-9,10-anthracenedione	28.8	27.4	1	1.0	443.2	477.9
1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)	26.3	24.0	1	2.0	382.1	371.1
1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene	27.5	29.7	1	4.0	360.6	373.3
1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene)	23.3	22.9	1	4.0	331.6	288.0
1,1'-(2,2-dichloroethylidenebis(4-chlorobenzene)	27.3	22.2	1	2.0	382.1	341.9
1,1,1-trichloroethane	10.1	9.9	3	0.0	240.1	241.3
1,1,1-trifluoro-n-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide	31.8	14.7	1	2.0	418.4	227.2
1,1,2,2-tetrachlorodifluoroethane	5.5	12.6	1	0.0	299.7	251.4
1,1,2,2-tetrachloroethane	9.7	12.4	1	1.0	230.8	216.6
1,1,2-trichloroethane	11.4	13.0	1	1.0	237.1	226.8
1,1,2-trifluoro-1,2,2-trichloroethane	4.9	10.8	1	0.0	236.9	215.8
1,10-decanediol	41.7	40.0	1	9.0	345.5	342.8
1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene	23.6	16.9	2	0.0	360.4	381.5
1,1-dichloroethane	7.9	8.0	1	0.0	176.2	159.5
1,1-difluoro-1-chloroethane	2.7	6.2	1	0.0	142.4	124.6
1,1-dimethyl-3-phenylurea	22.8	25.0	1	2.0	404.8	386.4
1,2,3,4-tetrachlorobenzene	17.0	13.7	2	0.0	320.0	308.5
1,2,3,4-tetrahydronaphthlene	12.5	16.0	1	1.0	237.4	279.3
1,2,3,5-tetrachlorobenzene	19.0	13.7	2	0.0	323.9	308.5
1,2,3,5-tetrafluorobenzene	10.7	9.6	1	0.0	226.9	192.4
1,2,3,6,7,8-hexahydropyrene	23.5	21.4	2	0.0	407.7	483.4
1,2,3-trichlorobenzene	20.5	12.6	2	0.0	326.9	285.2
1,2,3-trimethylbenzene	10.2	11.9	2	0.0	247.8	269.2
1,2,4,5-tetrabromobenzene	28.2	17.6	4	0.0	453.1	457.1
1,2,4,5-tetrachloro-3-nitrobenzene	19.5	17.1	1	0.0	373.3	341.7
1,2,4,5-tetrachlorobenzene	24.1	13.6	4	0.0	421.2	354.5
1,2,4,5-tetrafluorobenzene	15.1	9.6	4	0.0	277.0	249.9
1,2,4,5-tetramethylbenzene	20.9	12.7	4	0.0	352.4	329.9

1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene	28.9	22.5	1	0.0	419.9	450.0
1,2,4-trimethylbenzene	13.2	11.9	1	0.0	229.3	238.2
1,2:3,4-dibenzanthracene	25.8	23.7	2	0.0	553.5	534.5
1,2:5,6-dibenzanthracene	31.2	23.7	2	0.0	544.2	534.5
1,2-benzacenaphthene (fluoranthene)	18.7	16.9	1	0.0	383.4	338.9
1,2-benzanthracene	21.4	20.1	1	0.0	434.3	402.5
1,2-benzofluorene	22.2	19.0	1	0.0	462.8	380.8
1,2-benzopyrene	19.1	20.5	2	0.0	454.4	462.7
1,2-bromochlorobenzene	12.4	12.6	1	0.0	260.6	251.6
1,2-chloronitrobenzene	19.1	14.0	1	0.0	308.2	280.0
1,2-dibromobenzene	12.6	13.6	2	0.0	275.0	306.6
1,2-dibromoethane	13.1	15.2	1	1.0	283.0	265.6
1,2-dibromotetrafluoroethane	7.0	10.6	1	1.0	162.8	184.2
1,2-dicarbomethoxybenzene	17.0	20.3	1	2.5	274.2	295.9
1,2-dichlorobenzene	12.9	11.6	2	0.0	256.5	262.0
1,2-dichloroethane	8.8	13.6	1	1.0	237.2	237.0
1,2-dichloropropane	6.4	11.9	1	1.0	172.7	208.1
1,2-dichlorotetrafluoroethane	–	10.3	1	1.0	179.2	178.7
1,2-difluorobenzene	11.1	9.6	2	0.0	226.0	216.5
1,2-diiodobenzene	14.0	11.1	2	0.0	296.6	250.2
1,2-dinitrobenzene	22.8	16.4	2	0.0	396.1	370.7
1,2-diphenylethane	25.4	18.4	1	2.0	324.3	283.6
1,3,5-trichlorobenzene	18.2	12.6	6	0.0	336.7	359.2
1,3,5-trimethylbenzene	9.5	11.9	6	0.0	228.4	339.0
1,3,5-trinitro-1,3,5-triazacyclohexane	37.7	31.3	1	3.0	478.2	434.0
1,3,5-trinitrobenzene	16.7	19.8	1	0.0	380.3	396.8
1,3-bromochlorobenzene	12.3	12.6	1	0.0	252.0	251.6
1,3-butadiene	8.0	7.9	2	0.0	164.2	179.4
1,3-dibromobenzene	13.2	13.6	2	0.0	266.3	306.6
1,3-dibromopropane	14.6	18.2	1	2.0	238.6	280.8
1,3-dicarbomethoxybenzene	25.3	20.3	1	2.5	341.2	295.9
1,3-dichlorobenzene	12.6	11.6	2	0.0	248.4	262.0
1,3-difluorobenzene	9.4	5.2	2	0.0	204.0	116.5
1,3-diiodobenzene	15.9	6.6	2	0.0	307.4	150.2
1,3-dinitrobenzene	17.4	16.4	1	0.0	363.2	328.1
1,3-diphenylurea	34.6	31.8	1	2.0	512.0	490.1
1,3-nitrochlorobenzene	19.4	14.0	1	0.0	317.6	280.0
1,4-bromochlorobenzene	18.8	12.6	2	0.0	337.8	284.3
1,4-bromoiodobenzene	19.1	14.5	2	0.0	363.3	328.4
1,4-cyclohexadiene	6.5	12.2	2	0.0	224.0	276.0
1,4-diamino-2-methoxyanthraquinone	35.3	31.6	1	1.0	515.2	550.0
1,4-diaminoanthraquinone	24.2	27.7	2	0.0	484.2	626.1
1,4-dibromobenzene	20.0	13.6	4	0.0	360.1	352.4
1,4-dicarbomethoxybenzene	32.1	20.3	1	2.5	413.8	295.9
1,4-dichloro-2,5-dimethoxybenzene	27.6	19.3	1	1.5	403.9	316.1
1,4-dichlorobenzene	18.2	11.6	4	0.0	326.0	301.1
1,4-dihydroxybenzene	27.0	17.0	4	0.0	453.0	440.3
1,4-diiodobenzene	22.4	15.5	4	0.0	402.0	402.5
1,4-dimethylnaphthalene	10.6	14.6	2	0.0	279.9	331.0
1,4-dinitrobenzene	28.1	16.4	4	0.0	446.7	426.1

1,4-nitrochlorobenzene	11.9	14.0	2	0.0	354.6	316.3
1,4-pentadiene	6.1	3.4	1	1.0	124.3	58.5
1,5-dichloro-3-oxapentane	8.4	21.1	1	4.0	226.5	264.9
1,8-dimethylnaphthalene	15.8	14.6	2	0.0	336.3	331.0
10H-phenothiazine	26.9	24.9	1	0.0	458.2	497.7
17-methyltestosterone	–	20.1	1	0.0	438.0	401.0
1a,2a,3ß,4a,5a,6ß-hexachlorocyclohexane	22.1	22.6	1	3.0	386.8	313.2
1-aminoanthraquinone	28.8	25.5	1	0.0	524.2	509.7
1-bromo-2-chloroethane	14.0	14.4	1	1.0	256.4	251.3
1-bromobutane	9.2	15.3	1	2.0	160.4	235.9
1-bromoheptane	21.8	24.2	1	5.0	214.4	277.6
1-bromohexane	18.1	21.2	1	4.0	188.1	266.3
1-bromonaphthalene	15.2	15.1	1	0.0	271.4	301.6
1-bromooctane	24.7	27.1	1	6.0	218.2	287.1
1-bromopentane	14.4	18.2	1	3.0	185.1	252.6
1-butene	3.9	4.5	1	0.5	87.8	83.6
1-butyne	6.0	6.7	1	0.0	147.4	134.2
1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene	23.1	24.0	1	2.0	345.8	371.1
1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene	23.8	16.9	1	0.0	349.8	337.6
1-chlorodibenzodioxin	23.2	17.8	1	0.0	378.2	356.3
1-chloronaphthalene	12.9	14.1	1	0.0	270.7	281.9
1-decanol	37.7	33.6	1	8.0	280.1	307.3
1-decene	22.1	26.1	1	6.5	206.9	266.4
1-heptanethiol	25.4	21.3	1	5.0	229.9	245.1
1-heptanol	18.2	24.7	1	5.0	240.4	283.8
1-heptene	12.6	13.4	1	3.5	154.3	175.9
1-hexanol	15.5	13.8	1	4.0	225.8	173.1
1-hexene	9.4	10.4	1	2.5	133.4	151.7
1-iodonaphthalene	15.9	16.0	1	0.0	280.0	320.9
1-methylnaphthalene	12.0	13.9	1	0.0	242.7	277.1
1-naphthaleneacetamide	32.8	25.6	1	1.0	455.5	446.7
1-naphthaleneacetic acid	22.3	22.6	1	1.0	405.3	394.1
1-naphthoic acid	19.9	22.8	1	0.0	435.2	455.3
1-naphthyl methylcarbamate	24.5	24.9	1	2.0	416.3	383.8
1-naphthylamine	15.5	16.6	1	0.0	323.2	331.6
1-nitronaphthalene	18.4	16.5	1	0.0	329.9	330.0
1-nonene	20.0	19.3	1	5.5	191.6	212.3
1-octene	15.3	16.3	1	4.5	171.5	195.7
1-pentadecanol	54.7	48.3	1	14.0	316.6	314.7
1-propanethiol	9.9	9.5	1	1.0	160.0	165.7
1-tetradecanol	49.4	45.4	1	13.0	311.0	310.4
2-(1,3-dioxolan-2-yl)phenyl methylcarbamate	23.8	32.1	1	2.5	387.2	468.8
2-(1'-cyclohexenyl)cyclohexanone	17.3	23.9	1	7.5	278.8	226.9
2-(1-methylethyl)phenyl methylcarbamate	26.1	23.1	1	3.0	369.3	319.8
2-(2,4,5-trichlorophenoxy)propanoic acid	39.6	27.1	1	2.0	450.6	417.8
2-(2,4-dichlorophenoxy)propanoic acid	30.4	26.0	1	2.0	389.2	401.9
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	29.5	22.7	1	1.0	396.3	396.3
2-(4-chloro-2-methylphenoxy)propanoic acid	26.4	25.8	1	2.0	366.2	398.3

2-(6-methoxy-2-naphthyl)propionic acid	29.4	25.9	1	2.0	439.2	399.0
2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	22.6	24.0	2	0.0	455.8	542.1
2,2',3,3',5,5',6,6'-octachlorobiphenyl	22.8	23.0	4	0.0	433.8	596.3
2,2',3,3',5,5',6-heptachlorobiphenyl	20.3	21.9	1	0.0	395.4	438.6
2,2',3,3',6,6'-hexachlorobiphenyl	21.1	20.9	1	0.0	385.2	418.0
2,2',4,5,5'-pentachlorobiphenyl	18.8	19.9	1	0.0	350.1	397.4
2,2',4',5-tetrachlorobiphenyl	23.4	18.8	1	0.0	339.1	376.8
2,2,4-trimethylpentane	9.2	12.5	1	1.0	165.8	217.4
2,2-dimethyl-1-propanol	8.2	14.6	1	0.0	264.0	292.7
2,2-dimethylbutane	8.0	11.2	1	0.0	174.3	223.7
2,2-dimethylpentane	5.9	14.1	1	1.0	148.1	246.3
2,2-dimethylpropane	8.0	8.2	12	0.0	256.5	280.2
2,2-dimethylpropanoic acid (pivalic acid)	11.4	15.6	1	0.0	309.1	312.4
2,3,4,5,6-pentachlorobiphenyl	21.4	19.9	2	0.0	397.6	449.1
2,3,4,5-tetrachlorobiphenyl	25.2	18.8	1	0.0	363.9	376.8
2,3,4-trimethylpentane	9.3	7.4	1	2.0	163.6	114.2
2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione	30.9	23.3	4	0.0	567.2	605.8
2,3,6-trichlorophenylacetic acid	22.4	22.2	1	1.0	432.3	386.4
2,3-benzofluorene	23.4	19.0	1	0.0	489.7	380.8
2,3-dichloro-1,4-naphthalenedione	28.5	21.8	2	0.0	469.0	492.6
2,3-dichlorophenol	21.4	15.1	1	0.0	330.0	302.2
2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	30.3	26.8	1	2.0	426.2	412.9
2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	26.7	27.5	1	2.5	401.5	401.5
2,3-dimethylbutane	7.7	6.1	1	1.0	145.2	106.4
2,3-dimethylnaphthalene	15.9	14.6	2	0.0	378.0	331.0
2,3-dimethylphenol	21.0	14.8	1	0.0	346.0	296.5
2,3-dinitrotoluene	17.6	17.2	1	0.0	329.8	343.9
2,4,5,6-tetrachloro-1,3-benzenedicarbonitile	30.0	21.9	2	0.0	526.2	495.3
2,4,5-trichlorobiphenyl	22.8	17.8	1	0.0	349.5	356.3
2,4,5-trichlorophenol	21.6	16.1	1	0.0	340.3	322.8
2,4,6-N-tetranitroethylaniline	23.5	30.2	1	1.5	369.0	494.6
2,4,6-tribromophenol	18.5	18.9	1	0.0	366.2	378.2
2,4,6-trichlorobiphenyl	16.5	17.8	2	0.0	334.3	402.6
2,4,6-trimethyl-1,3,5-trioxane	15.5	18.0	1	0.0	285.7	359.7
2,4,6-trimethylpyridine	9.5	11.3	2	0.0	229.0	254.3
2,4,6-trinitroresorcinol	33.5	22.1	1	0.0	454.8	441.5
2,4,6-trinitrotoluene	23.4	20.6	2	0.0	352.2	466.2
2,4,6-tri-tert-butylphenol	19.5	23.0	1	0.0	405.2	460.7
2,4-dibromophenol	14.6	17.1	1	0.0	313.0	341.7
2,4-dichlorophenol	20.1	15.1	1	0.0	318.0	302.2
2,4-dichlorophenyl 4-nitrophenyl ether	23.0	21.3	1	1.0	342.0	371.6
2,4-dimethylpentane	6.9	9.1	1	2.0	154.0	139.8
2,4-dinitrochlorobenzene	20.2	17.4	1	0.0	325.2	348.7
2,4-dinitrophenol	24.2	18.8	1	0.0	388.0	376.4
2,4-dinitrotoluene	20.1	17.2	1	0.0	343.3	343.9
2,5-dichlorophenol	22.4	15.1	1	0.0	331.0	302.2
2,5-dimethylaniline	13.7	14.6	1	0.0	279.0	292.6
2,5-dimethylphenol	23.4	19.8	1	0.0	348.0	396.5
2,5-dinitrophenol	23.7	18.8	1	0.0	381.0	376.4

2,6-dichloro-4-benzenamine	29.5	15.1	2	0.0	467.2	341.4
2,6-dichloro-4-nitroaniline	32.6	18.2	2	0.0	466.8	410.4
2,6-dichlorobenzonitrile	26.2	15.7	2	0.0	417.2	355.4
2,6-dichlorobiphenyl	12.6	16.8	2	0.0	307.9	379.3
2,6-dichlorophenol	22.1	14.9	2	0.0	340.0	337.2
2,6-dimethylnaphthalene	25.1	14.6	2	0.0	383.3	331.0
2,6-dimethylphenol	18.9	14.8	2	0.0	318.9	335.1
2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	22.3	30.4	1	8.0	321.4	278.6
2,6-di-tert-butyl-4-methylphenol	23.9	20.6	1	0.0	343.7	411.0
2,6-di-tert-butylphenol	16.6	19.8	1	0.0	310.7	395.0
2,7-dimethylnaphthalene	23.4	14.6	2	0.0	368.8	331.0
2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	35.5	24.5	1	0.5	454.2	455.9
2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	38.0	28.4	1	2.0	476.0	438.7
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	42.0	37.3	1	3.5	437.9	491.3
2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	42.2	33.0	1	3.5	462.2	434.8
2-aminobenzoic acid	20.5	20.2	1	0.0	417.8	403.2
2-bromo-2-chloro-1,1,1-trifluoroethane	4.8	9.7	1	0.0	154.7	193.6
2-bromonaphthalene	20.3	15.1	1	0.0	329.0	301.6
2-bromopropane	6.6	7.7	1	0.0	184.1	154.5
2-butanethiol	6.5	7.9	1	1.0	133.0	136.8
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	30.1	26.6	1	5.0	358.8	305.4
2-chloro-6-(trichloromethyl)pyridine	20.3	16.3	1	0.0	337.8	325.2
2-chlorobenzoic acid	25.7	19.0	1	0.0	413.4	379.4
2-chlorobiphenyl	14.5	15.8	1	0.0	304.9	315.1
2-chlorodibenzodioxin	23.1	17.8	1	0.0	362.2	356.3
2-chloro-n-(2,6-diethylphenyl)-n-(methoxymethyl)acetamide	25.3	25.7	1	6.0	315.9	271.9
2-chloronaphthalene	14.7	14.1	1	0.0	332.0	281.9
2-chloro-N-isopropyl N-phenylacetamide	26.1	19.6	1	3.0	351.4	271.5
2-chlorophenol	12.6	14.1	1	0.0	283.0	281.6
2-chloropropane	7.4	6.9	1	0.0	156.0	138.1
2-cyclohexyl-4,6-dinitrophenol	28.0	28.0	1	2.5	378.7	408.1
2-heptanone	19.7	18.3	1	3.5	237.7	241.3
2-hexanone	14.9	15.4	1	2.5	217.7	224.2
2-hydroxybenzoic acid	24.6	20.4	1	0.0	431.8	407.1
2-iodobenzoic acid	21.4	20.9	1	0.0	435.1	418.4
2-isopropoxyphenyl N-methylcarbamate	23.0	26.5	1	4.0	363.1	332.9
2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide	16.9	17.3	1	0.5	327.9	322.2
2-methyl-1,3-butadiene	4.9	6.9	1	0.0	127.3	138.2
2-methyl-1-butene	7.9	6.8	1	0.5	135.6	126.7
2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime	22.7	29.5	1	4.5	374.0	353.7
2-methyl-2-butene	7.6	7.5	1	0.0	139.4	149.1
2-methyl-4,6-dinitrophenol	19.4	9.6	1	0.0	359.3	192.2
2-methylbutane	5.1	6.9	1	1.0	113.4	120.5
2-methylfuran	8.6	9.7	1	0.0	181.9	193.9
2-methylheptane	–	16.6	1	4.0	168.2	208.9
2-methylhexane	9.2	13.7	1	3.0	154.9	189.4

2-methylnaphthalene	18.1	13.9	1	0.0	307.7	277.1
2-methylpentane	6.3	10.7	1	2.0	119.6	165.4
2-naphthoic acid	23.5	22.8	1	0.0	460.2	455.3
2-naphthylamine	23.3	16.6	1	0.0	386.2	331.6
2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	18.4	22.2	1	4.0	364.6	278.4
2-nitro-5-methylphenol	20.8	16.2	1	0.0	302.8	323.5
2-nitroaniline	16.1	15.2	1	0.0	344.4	303.8
2-octanone	24.4	21.3	1	4.5	252.9	255.3
2-pentanol	8.5	14.1	1	2.0	200.0	217.8
2-pentanone	11.1	12.4	1	1.5	196.3	203.0
2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate	18.9	32.3	1	5.0	341.3	371.4
3-(3,4-dichlorophenyl)-1,1-dimethylurea	33.9	27.1	1	2.0	429.7	418.2
3-(4-chlorophenyl)-1,1-dimethylurea	29.5	26.1	1	2.0	447.6	402.3
3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	25.5	24.2	1	1.5	408.9	396.6
3(n-octyloxy)-1,2-propanediol	33.4	39.8	1	10.0	296.1	321.2
3-(p-tolyl-4-sulfonyl)-1-butyl urea	25.6	33.2	1	5.0	404.8	382.0
3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime	19.8	26.8	1	4.5	330.2	321.2
3,3-dimethyl-2-butanone	11.3	11.3	1	0.0	221.7	226.1
3,3-dimethylpentane	7.1	7.7	1	2.0	138.2	118.2
3,3'-di-tert-butyl-5,5'-dimethyl-2,2-dihydroxydiphenylmethane	29.3	31.8	1	3.0	403.7	440.6
3,4-benzophenanthrene	16.3	20.1	1	0.0	334.7	402.5
3,4-benzopyrene	27.2	20.5	1	0.0	454.2	409.5
3,4-dichloro-2-methoxybenzoic acid	35.3	23.7	1	1.0	412.5	412.4
3,4-dichlorophenol	20.9	15.3	1	0.0	341.0	306.0
3',4'-dichloropropionanilide	18.3	24.2	1	2.0	363.7	372.7
3,4-dimethylisoxazol 5-sulphanylamide	28.0	26.9	1	1.0	448.2	467.9
3,4-dimethylphenol	18.1	19.8	1	0.0	334.0	396.5
3,4-dimethylphenyl methylcarbamate	25.0	22.9	1	2.0	350.8	353.7
3,4-dinitrotoluene	18.8	17.2	1	0.0	329.5	343.9
3,5,6-trichloro-2-pyridinyloxyacetic acid	31.2	27.5	1	2.0	423.3	425.0
3,5-dibromo-4-hydroxybenzonitrile	32.0	21.0	2	0.0	464.0	475.2
3,5-dichlorobenzoic acid	23.0	21.3	2	0.0	459.3	481.2
3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	28.7	26.5	1	2.0	428.4	409.7
3,5-dichlorophenol	20.5	15.3	2	0.0	341.0	345.8
3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate	18.4	25.7	1	3.0	361.7	355.6
3,5-dimethylphenol	18.0	14.8	2	0.0	336.8	335.1
3,5-dinitrobenzoic acid	22.8	26.1	1	0.0	480.4	522.1
3,6-dichloro-2-methoxybenzoic acid	22.9	23.7	1	1.0	386.7	412.4
3-amino-2,5-dichlorobenzoic acid	37.4	23.3	1	0.0	475.6	466.4
3-aminobenzoic acid	21.8	22.8	1	0.0	452.9	455.0
3-chlorobenzoic acid	23.9	20.3	1	0.0	427.4	405.3
3-chlorophenol	14.9	14.3	1	0.0	305.8	285.4
3-heptanone	17.5	16.0	1	3.5	236.0	210.5
3-hexanone	14.5	13.0	1	2.5	217.7	190.1
3-hydroxybenzoic acid	26.2	22.9	1	0.0	475.1	458.9
3-iodobenzoic acid	28.7	22.2	1	0.0	460.4	444.3
3-methyl-1-butene	5.4	4.8	1	0.5	104.7	89.9

3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	21.4	24.4	1	2.0	324.3	376.7
3-methylheptane	11.7	16.6	1	4.0	152.6	208.9
3-methylpentane	5.3	10.7	1	2.0	110.3	165.4
3-methylthiophene	10.5	10.3	1	0.0	204.2	206.8
3-nitroaniline	23.7	16.5	1	0.0	387.2	329.7
3-nitrotoluene	15.0	13.8	1	0.0	288.7	275.2
3-pentanol	9.1	14.1	1	2.0	204.2	217.8
3-pentanone	11.7	10.1	1	1.5	234.2	164.8
4-(1,1-dimethylethyl)-n-(1-methylpropyl)-2,6-dinitrobenzeneamine	20.8	26.8	1	6.0	338.8	283.9
4-(2,4,5-trichlorophenoxy)butanoic acid	30.3	32.7	1	4.0	386.7	410.2
4-(2,4-dichlorophenoxy)butyric acid	38.4	31.6	1	4.0	391.4	397.2
4-(4-chloro-2-methylphenoxy)butanoic acid	32.0	31.4	1	4.0	373.4	394.3
4-(4-nitrophenylazo)aniline	31.9	22.8	1	1.0	488.2	396.4
4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide	38.5	33.2	1	4.5	414.8	398.3
4,4'dihydroxydiphenyl-2,2-propane	30.1	22.1	1	1.0	433.0	384.9
4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	31.5	23.0	1	1.0	431.0	400.1
4-aminoacetophenone	38.0	17.2	1	0.0	379.2	344.4
4-aminobenzoic acid	20.9	22.7	2	0.0	461.4	514.1
4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide	22.3	30.3	1	2.0	453.4	466.9
4-aminopyridine	20.1	13.9	2	0.0	429.9	313.0
4-bromophenol	0.0	15.3	2	0.0	336.0	344.8
4-chloroazobenzene	27.2	16.8	2	0.0	361.2	380.2
4-chlorobenzoic acid	32.3	20.3	2	0.0	512.9	457.9
4-chlorobiphenyl	13.3	15.8	2	0.0	348.6	356.0
4-chlorophenol	14.1	14.3	2	0.0	315.9	322.2
4-chlorophenoxyacetic acid	36.3	24.7	1	2.0	429.6	380.8
4-heptanone	16.2	16.0	1	3.5	240.2	210.5
4-hexylresorcinol	19.0	30.2	1	4.5	341.5	362.4
4-hydroxy-3,5-diiodobenzonitrile	33.6	23.0	2	0.0	482.9	518.8
4-hydroxyazobenzene	33.0	19.5	2	0.0	425.2	440.8
4-hydroxybenzoic acid	30.9	22.9	2	0.0	488.1	518.5
4-hydroxyphenylacetic acid	28.4	22.8	1	1.0	423.6	397.2
4-iodobenzoic acid	35.2	22.2	2	0.0	543.8	502.1
4-methoxybenzoic acid	28.4	23.1	1	1.0	457.8	402.4
4-methoxyphenol	18.3	17.1	1	0.5	328.4	318.5
4-methoxyphenylpropionic acid	28.5	25.1	1	3.0	376.9	347.1
4-methylpent-1-ene	4.9	5.8	1	1.5	118.9	94.7
4-methylphenanthrene	14.1	17.4	1	0.0	324.9	347.1
4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline	28.1	36.0	1	5.0	424.3	413.6
4-methylthio-3,5-xylyl methylcarbamate	30.4	26.3	1	3.0	393.8	364.7
4-nitro-5-methylphenol	27.4	17.5	1	0.0	401.0	349.4
4-nitroaniline	21.1	16.5	2	0.0	420.2	372.5
4-nitrotoluene	16.8	13.8	2	0.0	324.8	311.0
4-oxaheptane	10.8	16.9	1	4.0	158.4	212.3
4-tert-butylbenzoic acid	17.9	22.5	1	0.0	440.0	450.0
4-tert-butylphenol	14.5	16.5	1	0.0	373.2	330.1
5'-(trifluoromethanesulphonamide)acet-2',4-xylidide	37.7	31.6	1	2.0	457.3	487.0
5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-	22.0	25.1	1	1.5	428.3	411.1

pyrimidinedione						
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	12.5	23.5	1	0.0	448.0	469.0
5-isopropyl-m-tolyl methylcarbamate	23.0	23.9	1	3.0	361.3	330.8
5-methyl N-(methylcarbamoyloxy)thioacetimidate	21.7	26.7	1	3.5	352.7	351.9
5-methyl-1,2,4-triazolo[3,4-b]benzothiazole	24.1	17.2	1	0.0	460.2	343.5
5-nonanone	26.2	21.9	1	5.5	223.2	241.3
acenaphthene	21.5	14.9	2	0.0	366.6	336.7
acenaphthylene	–	13.3	2	0.0	368.2	300.7
acetohexamide	–	37.6	1	6.0	461.2	398.1
acetylene	7.2	8.9	2	0.0	192.4	200.8
acridine	18.6	17.4	2	0.0	383.2	393.1
adipic acid	34.9	29.9	1	4.0	426.4	376.1
aldicarb	–	29.5	1	4.5	372.2	353.7
aldoxycarb	–	36.2	1	4.0	414.2	454.7
allobarbitiol	32.3	26.6	1	2.5	442.6	389.0
a-methylstyrene	11.9	10.0	1	0.0	250.8	200.5
ametryn	–	28.8	1	3.5	358.2	379.3
aminocarb	–	24.9	1	3.0	367.2	344.6
amobarbital	–	34.9	1	4.5	429.2	418.5
a-naphthol	23.0	16.8	1	0.0	369.0	335.5
a-naphthyl acetate	20.2	22.6	1	1.0	319.2	394.1
aniline	10.5	13.0	2	0.0	267.1	294.9
anthracene	29.4	16.6	4	0.0	488.9	431.1
anthraquinone	32.6	23.3	4	0.0	558.0	604.4
aprobarbital	–	27.8	1	3.0	414.2	385.3
atrazine	–	30.3	1	3.5	448.2	399.5
azelaic acid	32.7	38.8	1	7.0	380.0	381.2
b(4-chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	24.5	32.9	1	4.0	377.8	413.5
barbital	25.0	30.6	1	1.5	462.6	500.8
bendiocarb	–	28.7	1	2.0	403.2	443.6
bendroflumethiazide	–	29.9	1	1.0	495.2	520.8
benfluralin	–	30.4	1	4.5	339.2	365.1
benzaldehyde	–	14.7	1	0.0	247.2	293.0
benzamide	18.5	20.0	1	0.0	402.3	399.6
benzene	9.9	9.5	12	0.0	278.7	324.4
benzidine	19.1	21.8	4	0.0	400.2	565.0
benzimidazole	19.3	19.0	2	0.0	443.2	428.6
benzofluoranthene	18.5	17.4	1	0.0	424.0	348.9
benzoic acid	18.0	19.2	2	0.0	395.5	434.7
benzonitrile	11.0	13.7	2	0.0	260.3	308.9
benzophenone	18.4	14.5	2	0.0	324.2	328.8
benzothiazole	12.8	13.9	1	0.0	275.6	277.6
benzothiophene	11.8	13.1	1	0.0	304.5	261.6
benzotrifluoride	13.8	9.0	1	0.0	244.0	179.4
benzoxazole	16.8	12.4	1	0.0	302.5	247.5
benzyl alcohol	8.8	14.4	1	0.5	257.6	268.1
betamethasone	–	28.0	1	0.5	503.0	520.9
betamethasone-17-valerate	–	37.5	1	5.0	456.0	431.6
beta-naphthol	18.8	16.8	1	0.0	393.6	335.5

biphenyl	18.7	14.7	4	0.0	341.5	382.5
bis-(4-aminophenyl)methane	9.2	23.3	1	1.0	363.7	405.8
bromobenzene	10.7	11.5	2	0.0	242.4	261.0
bromocyclohexane	10.8	16.2	1	3.0	216.9	225.0
bromomethane	6.0	6.4	1	0.0	179.5	128.6
butacarb	–	27.9	1	2.0	376.2	430.1
butalbital	–	30.8	1	4.0	412.2	386.7
butanal	11.1	12.4	1	1.5	176.8	202.2
butane	7.2	9.4	1	1.0	134.9	164.2
butanoic acid	11.1	16.7	1	1.5	264.7	273.7
butocarboxim	–	24.6	1	4.5	298.2	295.5
butyl 4-aminobenzoate	20.5	27.3	1	4.0	331.1	342.7
butyl 9-hydroxy-9H-fluorene-9-carboxylate	25.6	25.7	1	4.0	343.9	323.1
butyl acrylate	17.3	20.6	1	4.0	209.5	259.4
butyl alcohol	9.3	15.8	1	2.0	183.9	244.2
butyl benzyl phthalate	–	26.4	1	7.0	238.2	259.2
butyl butanoate	14.9	21.5	1	5.5	181.7	236.8
caffeine	24.4	26.3	1	0.0	512.0	526.5
carbaryl	–	24.9	1	2.0	418.2	383.8
carbazole	26.9	21.7	2	0.0	516.0	490.2
carbendazim	–	30.8	1	2.0	523.2	474.9
carbon tetrabromide	10.7	12.4	12	0.0	363.2	421.1
carbon tetrachloride	7.8	9.1	12	0.0	249.0	309.6
carbon tetrafluoride	2.4	1.8	12	0.0	89.6	62.0
chlorimuron	–	43.7	1	6.5	454.2	445.8
chlorobenzene	–	10.6	2	0.0	228.0	238.7
chlorocyclohexane	10.5	15.4	1	3.0	229.3	213.7
chlorodifluoromethane	4.2	2.8	1	0.0	115.7	56.1
chloroethane	4.5	8.6	1	0.0	134.8	171.2
chlorothiazide	–	30.5	1	0.0	616.2	610.5
chlorotoluron	–	26.9	1	2.0	421.2	414.5
chloroxuron	–	32.4	1	3.5	424.2	426.6
chlorpropamide	–	30.5	1	4.5	400.2	366.3
chlorsulfuron	–	32.4	1	4.0	449.2	406.5
cholesterol	30.9	30.0	1	4.0	421.0	376.7
chrysene	29.4	20.1	2	0.0	531.4	454.8
cinnamic acid	22.6	24.6	1	1.0	406.2	428.2
cis-1,2-dimethylcyclohexane	12.3	12.7	1	3.0	223.3	175.6
cis-1,4-dimethylcyclohexane	9.3	12.7	1	3.0	185.7	175.6
cis-2-butene	7.3	5.1	2	0.0	134.3	116.2
cis-2-hexene	8.9	8.7	1	2.0	132.0	134.5
cis-2-pentene	7.1	5.8	1	1.0	121.8	100.4
cis-crotonic acid	12.6	17.4	1	0.5	344.4	323.9
coronene	19.2	21.2	12	0.0	710.5	720.7
cortisone	36.9	24.5	1	0.5	495.0	456.7
cortisone acetate	38.4	32.0	1	2.0	509.0	493.5
coumarin	19.1	17.9	1	0.0	342.1	358.5
cyanazine	–	37.3	1	3.5	440.2	491.3
cycloate	–	27.8	1	6.5	284.7	283.8
cycloheptane	12.6	16.3	1	4.0	265.1	205.1

cycloheptanol	–	12.0	1	0.0	275.2	239.6
cycloheptatriene	3.5	11.5	1	1.0	198.0	201.1
cycloheptene	9.1	14.7	1	3.0	217.0	204.0
cyclohexane	12.8	14.0	1	3.0	279.8	193.8
cyclohexanol	11.7	16.7	1	3.0	297.0	231.8
cyclohexanone	10.9	15.9	1	2.5	245.2	232.7
cyclohexene	8.5	12.4	1	2.0	169.7	191.3
cyclooctane	14.1	18.7	1	5.0	288.0	214.5
cyclopentane	8.3	11.7	1	2.0	179.7	179.9
cyclopentene	4.1	10.1	1	1.0	138.1	175.3
cyclopropane	5.4	7.0	6	0.0	145.6	198.9
cyprazine	–	30.2	1	2.5	440.2	440.2
dacthal	–	24.4	1	2.5	428.2	356.1
daimuron	–	36.5	1	3.5	476.2	481.1
decachlorobiphenyl	39.3	25.0	4	0.0	577.7	649.8
decanoic acid	27.8	34.5	1	7.5	304.5	326.6
deoxycorticosterone	28.0	25.5	1	0.5	414.0	475.7
deoxycorticosterone acetate	29.7	26.1	1	2.0	430.0	402.6
desmetryn	–	25.8	1	3.5	358.2	340.4
dexamethasone	42.0	28.0	1	0.5	539.0	520.9
diallate	–	21.7	1	5.5	298.2	239.3
dibenzodioxin	23.2	16.8	4	0.0	395.7	435.9
dibenzofuran	18.6	15.1	2	0.0	355.7	341.2
dibutyl phthalate	–	38.0	1	8.5	238.2	336.6
dichloromethane	6.2	9.6	1	0.0	178.2	192.7
diethyl disulfide	9.4	15.1	1	3.0	171.6	208.5
diethyl ether	7.2	11.0	1	2.0	156.9	169.7
diethyl o-phthalate	18.0	26.2	1	4.5	269.9	314.3
diethyl phthalate	–	26.2	1	4.5	270.2	314.3
diethyl sulfide	11.9	12.2	1	2.0	169.2	188.9
diethylstilbestrol	31.6	27.6	1	3.0	442.0	382.3
difenoxuron	–	35.2	1	4.5	412.2	422.8
diflubenzuron	–	32.7	1	3.0	512.2	452.6
diiodomethane	12.1	15.1	1	0.0	279.2	302.0
diisopropyl ketone	11.2	10.7	1	1.5	204.8	175.9
dimepiperate	–	29.5	1	5.0	312.2	339.5
dimetan	–	23.4	1	3.0	318.7	324.1
dimethametryn	–	30.1	1	5.5	338.2	331.7
dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	25.0	24.9	1	2.0	384.0	384.0
dimethyl fumarate	35.2	21.0	1	3.0	375.0	290.5
dimethyl maleate	14.6	21.0	1	3.0	254.0	290.5
dimethyl oxalate	21.1	29.5	1	2.0	327.6	455.9
dimethyl phthalate	–	20.3	1	2.5	275.2	295.9
dimethyl sulfide	8.0	6.3	1	0.0	174.9	126.7
dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	30.2	24.4	1	2.5	431.7	356.1
di-n-butyl succinate	29.2	33.5	1	10.0	244.1	270.4
diphenyl ether	17.2	15.8	1	1.0	300.0	275.9
diphenyl phthalate	–	30.9	1	3.5	345.2	407.5
diphenylacetic acid	31.3	23.8	1	1.0	420.4	414.4
diphenylamine	17.9	21.1	1	1.0	326.2	367.1

diphenylcarbinol	23.0	19.0	1	1.0	338.5	331.6
diphenylmethane	18.6	16.3	1	1.0	298.3	283.4
dipropalin	–	31.8	1	4.5	353.2	381.3
Dipropetryn	–	30.1	1	5.5	378.2	331.7
diuron	–	27.1	1	2.0	432.2	418.2
d-limonene	11.4	14.8	1	1.5	199.2	242.9
dodecane	36.8	33.1	1	9.0	263.6	283.5
dodecanedioic acid	50.6	47.7	1	10.0	402.5	384.5
dodecanol	40.2	39.5	1	10.0	300.2	318.3
E-3-chloro-2-butenoic acid	13.8	19.9	1	0.5	333.7	371.3
estradiol	0.0	23.6	1	0.0	452.0	471.0
estrone	48.0	22.8	1	0.0	533.2	455.1
ethalfluralin	–	24.8	1	3.0	332.2	343.9
ethane	2.8	3.5	20	0.0	89.5	140.0
ethiofencarb	–	28.5	1	5.0	306.6	327.9
ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	32.8	41.4	1	5.0	394.1	476.2
ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	23.5	26.2	1	3.0	310.4	363.2
ethyl 4-aminobenzoate	23.6	21.4	1	2.0	362.8	329.8
ethyl acetate	10.5	12.0	1	1.5	189.3	196.3
ethyl mercaptan	5.0	6.6	1	0.0	195.3	131.1
ethyl N-benzoyl-n-(3,4-dichlorophenyl)-dl-alaninate	27.1	27.6	1	4.0	341.7	347.0
ethyl nitrate	8.5	8.7	1	0.0	178.6	174.4
ethyl propyl ether	8.4	13.9	1	3.0	145.7	193.2
ethylbenzene	9.2	10.9	1	0.5	178.2	203.8
ethylcyclohexane	8.3	16.3	1	3.5	161.4	214.6
ethylene	3.4	1.7	20	0.0	104.0	67.6
ethynyl estradiol	–	17.5	1	0.0	456.2	349.8
fenobucarb	–	26.0	1	4.0	304.7	327.2
fenothiocarb	–	33.8	1	7.0	313.7	332.1
fenuron	–	25.0	1	2.0	406.2	386.4
flazasulfuron	–	38.5	1	5.0	441.2	442.3
flufenoxuron	–	38.5	1	4.5	444.2	461.6
flumethiazide	–	28.9	1	0.0	573.2	578.7
fluometuron	–	24.5	1	2.0	437.2	377.7
fluorene	19.6	15.5	2	0.0	387.9	350.5
fluorobenzene	11.3	9.6	2	0.0	230.9	216.0
fluorotrichloromethane	6.9	7.3	3	0.0	162.7	178.1
forchlorfenuron	–	33.6	1	2.5	440.2	490.4
furan	–	8.0	2	0.0	187.6	181.7
furfural	14.4	12.3	1	0.0	235.1	246.6
glyburide	–	59.5	1	10.5	442.2	465.6
glyceryl triacetate	25.8	27.3	1	6.5	275.3	278.2
Halosulfuron	–	41.2	1	6.5	449.2	419.5
heptabarbital	–	39.3	1	4.5	447.2	472.0
heptanal	22.9	21.2	1	4.5	229.3	254.7
heptane	14.0	18.3	1	4.0	182.6	229.7
heptanoic acid	17.8	25.6	1	4.5	265.8	307.2
hexachlorobenzene	23.9	15.7	12	0.0	505.0	534.5
hexachloroethane	24.4	16.2	6	0.0	458.0	461.3
hexadecane	53.4	44.9	1	14.0	291.1	292.2

hexaflumuron	–	42.6	1	6.0	476.7	451.7
hexafluoroethane	8.9	5.3	20	0.0	173.1	210.6
hexamethylbenzene	22.4	14.3	12	0.0	438.7	486.1
hexanal	15.4	18.3	1	3.5	243.2	240.6
hydrochlorothiazide	–	29.6	1	0.0	547.2	592.2
hydrocinnamic acid	17.7	21.2	1	2.0	321.2	327.2
hydrocortisone	35.8	30.7	1	0.5	485.0	571.6
hydrocortisone-21-acetate	37.0	32.8	1	2.0	497.0	505.7
hydroflumethiazide	–	28.0	1	0.0	543.7	560.4
imazosulfuron	–	43.7	1	5.0	456.2	502.7
iodomethane	9.1	8.3	3	0.0	206.8	204.1
ipazine	–	28.4	1	4.5	360.2	340.6
isobutane	4.6	4.8	3	0.0	113.7	117.7
isobutene	5.9	6.2	2	0.0	132.4	139.7
isonicotinic acid	32.1	20.0	2	0.0	593.0	452.8
isoprocarb	–	23.1	1	3.0	367.2	319.8
isopropyl 4,4'-dibromobenzilate	24.6	26.5	1	3.0	348.1	367.5
isopropyl ether	12.1	7.7	1	2.0	187.8	118.5
isopropyl methyl ketone	9.3	9.8	1	0.5	180.0	182.3
isopropyl nitrate	10.1	10.5	1	0.0	190.9	209.9
isopropyl phenylcarbamate	19.4	22.6	1	3.0	359.5	313.5
isopropylbenzene	7.3	11.3	1	0.5	177.1	210.1
isoproturon	–	26.8	1	3.0	431.2	371.1
isoquinoline	13.5	13.9	1	0.0	299.6	277.3
isouron	–	26.8	1	2.0	392.7	414.0
L-carvone	11.6	16.8	1	0.0	247.7	335.7
linuron	–	26.4	1	3.0	367.2	365.0
lufenuron	–	44.3	1	6.0	439.2	469.1
m-acetotoluidide	–	22.3	1	1.0	339.2	387.8
m-aminophenol	23.0	16.8	1	0.0	399.0	335.1
m-benzenedicarboxylic acid	–	28.9	2	0.0	621.2	653.9
m-bromobenzoic acid	–	21.3	1	0.0	428.2	425.0
m-bromophenol	15.1	15.3	1	0.0	306.2	305.2
m-bromotoluene	–	12.3	1	0.0	233.2	246.8
m-chloroaniline	–	14.1	1	0.0	263.2	281.5
m-chlorotoluene	–	11.4	1	0.0	225.2	227.1
m-cyanoaniline	–	17.2	1	0.0	326.2	343.6
m-cymene	–	12.1	1	0.5	209.5	224.8
m-diethylbenzene	–	12.4	1	1.5	189.3	202.2
mebendazole	–	35.8	1	3.0	561.7	495.8
methabenzthiazuron	–	31.8	1	2.0	393.2	491.4
methanethiol	6.1	3.6	3	0.0	150.2	88.2
methiocarb	–	26.3	1	3.0	393.2	364.7
methomyl	–	26.7	1	3.5	351.2	351.9
methoxybenzene	14.1	13.4	1	0.5	293.2	249.4
methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	27.1	28.2	1	4.0	314.4	354.8
methyl 2,4-dichlorophenoxyacetate	25.1	21.6	1	3.0	315.4	299.1
methyl 3-m-tolylcarbamoyloxyphenylcarbamate	39.6	39.3	1	4.0	423.8	493.3
methyl 4-aminobenzoate	22.6	18.4	1	1.0	385.1	320.8
methyl 4-hydroxybenzoate	24.3	18.6	1	1.0	398.5	324.2

methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	26.3	26.7	1	3.0	358.3	369.9
methyl acrylate	9.7	11.8	1	1.0	197.5	205.3
methyl benzoate	13.9	14.9	1	1.0	261.0	259.6
methyl chloride	6.4	5.6	10	0.0	174.5	181.6
methyl isopropyl ether	5.9	6.4	1	1.0	127.3	111.2
methyl methacrylate	12.2	10.8	1	1.0	225.0	187.4
methyl n-butyl ether	10.9	13.9	1	3.0	157.5	193.2
methyl propyl ether	7.7	11.0	1	2.0	134.0	169.7
methyl tert-butyl ether	7.6	9.8	1	0.0	164.6	196.1
methylcyclohexane	6.7	13.3	1	3.0	146.6	184.7
methylcyclopentane	6.9	11.0	1	2.0	130.7	169.8
methyldymron	–	34.3	1	3.5	345.2	452.3
methylphenylsulfide	14.9	12.9	1	0.5	256.4	241.0
methylprednisolone	–	28.4	1	0.5	513.2	529.0
metobromuron	–	26.3	1	3.0	369.2	364.4
metolcarb	–	22.1	1	2.0	349.7	341.5
metoxuron	–	29.9	1	3.0	399.7	414.6
m-fluorobenzoic acid	–	19.3	1	0.0	397.2	385.1
m-hydroxybenzaldehyde	–	16.7	1	0.0	381.2	333.5
m-hydroxybenzyl alcohol	–	18.1	1	0.5	346.2	337.1
m-hydroxytoluene	10.7	14.0	1	0.0	285.4	280.7
m-nitrobenzaldehyde	–	16.4	1	0.0	331.2	328.0
m-nitrobenzoic acid	19.3	22.7	1	0.0	414.3	453.4
m-nitrobenzyl alcohol	–	17.8	1	0.5	300.2	332.0
m-nitrobromobenzene	–	15.0	1	0.0	329.2	299.7
m-nitrophenol	19.2	16.7	1	0.0	371.2	333.6
monuron	–	26.1	1	2.0	443.7	402.3
m-terphenyl	22.6	19.9	2	0.0	360.0	450.1
m-toluic acid	15.7	20.0	1	0.0	381.9	400.5
m-toluidine	8.8	13.8	1	0.0	241.7	276.8
m-xylene	11.6	11.1	2	0.0	225.3	251.3
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	25.2	28.1	1	6.0	327.5	297.3
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine	23.1	32.5	1	4.5	318.4	390.2
N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	29.1	26.7	1	2.5	372.1	390.1
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	32.0	22.7	1	1.5	395.5	371.2
N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea	27.5	29.9	1	3.0	399.2	414.6
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	16.4	30.2	1	4.0	353.2	378.9
N-(4-chlorophenyl)-2,2-dimethylpentanamide	23.3	30.9	1	4.0	360.2	388.1
N'-(4-chlorophenyl)-N-methoxy-N-methylurea	22.5	25.3	1	3.0	353.4	350.7
N-(cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl)benzenamine	22.5	20.1	1	7.0	305.8	197.5
N,N'-(2-hydroxyethyl)-1,4-diaminoanthraquinone	32.3	50.3	1	6.0	521.2	533.1
N,N-(2-hydroxyethyl)-4-phenylazoaniline	30.0	37.3	1	5.0	407.0	428.4
N,N-diethyl-2-(1-naphthyloxy)propionamide	24.6	30.6	1	5.0	345.3	351.2
N,N-dimethyl-2,2-diphenylacetamide	25.4	20.9	1	2.0	407.1	322.1
N,N-dimethyl-4-phenylazoaniline	23.1	18.5	1	1.0	389.2	323.1
N,N-dimethylaniline	12.8	15.5	1	0.5	275.6	288.7
N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea	29.8	27.6	1	2.0	434.1	426.4
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea	33.9	26.8	1	3.0	430.5	371.1

N,N'-dinitroethanediamine	29.5	29.7	1	3.0	450.0	412.0
N,N'-di-n-propyladipamide	36.1	47.8	1	10.0	452.0	385.1
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	43.1	27.9	1	2.0	432.0	430.6
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-propanamide (sufentanil)	23.9	40.7	1	6.0	370.2	430.7
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea	29.5	28.0	1	2.0	435.3	431.5
naphthalene	19.1	13.1	4	0.0	353.4	339.3
n-butyl mercaptan	10.5	12.5	1	2.0	157.5	192.3
n-butylbenzene	11.2	16.9	1	2.5	185.3	246.0
N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea	27.2	36.0	1	5.0	374.3	413.4
N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline	36.5	30.4	1	8.0	338.5	278.6
n-decane	28.7	27.2	1	7.0	243.5	266.7
n-hexane	13.1	15.3	1	3.0	177.8	212.3
nicosulfuron	–	40.3	1	6.5	415.2	410.9
nicotinic acid	27.5	20.0	1	0.0	510.0	400.8
nitralin	–	36.0	1	4.5	425.2	432.0
nitrobenzene	12.1	13.0	2	0.0	278.8	293.1
nitroethane	9.9	8.7	1	0.0	183.7	174.4
N-methyl-2,4,6,N-tetranitroaniline	25.9	27.3	1	0.5	402.6	507.7
n-octane	20.7	21.2	1	5.0	216.4	244.1
n-octylbenzene	30.0	28.7	1	7.0	234.2	281.7
nonanal	29.6	27.1	1	6.5	253.9	276.5
nonane	21.8	24.2	1	6.0	219.7	256.3
nonanoic acid	26.3	31.5	1	6.5	285.5	321.1
norethindrone	–	19.9	1	0.0	479.0	397.1
norethindrone acetate	–	22.9	1	0.5	480.0	426.2
novaluron	–	44.8	1	7.0	450.7	440.3
n-pentadecane	43.8	41.9	1	13.0	283.1	286.8
N-phenyl-N[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)	22.5	36.2	1	4.0	357.2	454.7
n-propylbenzene	9.3	13.9	1	1.5	173.6	227.5
N-Sulfanilylsulfanilamide	–	29.0	1	2.0	407.2	447.0
N-tert-butylurea	33.2	24.0	1	0.5	449.8	447.8
n-tridecane	36.5	36.0	1	11.0	267.8	274.1
n-undecane	29.4	30.1	1	8.0	247.6	275.7
O-(2-chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate	29.1	21.6	1	2.5	323.9	315.1
O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate	31.2	21.2	1	2.5	325.3	309.4
O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphonothioate	31.4	22.3	1	2.0	345.6	344.2
O,O-diethyl O-4-nitrophenyl phosphorothioate	15.7	26.5	1	4.5	278.1	317.7
O,O-diethyl O-quinoxalin-2-yl phosphothioate	25.4	28.2	1	4.5	304.1	338.2
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	24.5	26.9	1	4.5	315.0	323.2
O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	30.6	35.1	1	8.0	310.4	321.8
O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	18.9	20.2	1	2.5	313.0	295.0
O,O-dimethyl O-4-nitrophenyl phosphorothioate	20.1	20.6	1	2.5	308.2	300.1

O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate	20.5	25.5	1	4.5	321.0	306.1
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	25.9	21.0	1	2.5	318.7	306.7
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl O,O-diethyl phosphorothioate	27.3	35.9	1	7.0	324.4	353.1
o-acetoxybenzoic acid	–	22.8	1	1.0	408.2	396.8
o-aminophenol	34.0	16.4	1	0.0	447.4	327.5
o-benzenedicarboxylic acid	–	27.7	2	0.0	507.2	624.9
o-bromobenzoic acid	–	20.0	1	0.0	423.2	399.1
o-bromobenzyl alcohol	–	15.1	1	0.5	353.2	281.5
o-chloroacetanilide	–	16.6	1	1.0	361.2	288.6
o-chloroaniline	–	13.9	1	0.0	274.2	277.7
o-chloroanisole	–	14.4	1	0.5	246.4	268.6
o-chlorotoluene	–	11.4	1	0.0	235.2	227.1
octafluoropropane	5.0	9.5	1	0.0	125.5	190.7
octanal	25.9	24.2	1	5.5	288.2	266.5
octanoic acid	21.4	28.5	1	5.5	289.7	314.7
o-cymene	–	12.1	1	0.5	201.7	224.8
o-diethylbenzene	–	12.4	1	1.5	242.0	202.2
O-ethyl O-(4-nitrophenyl)phenylphosphonothioate	25.1	24.6	1	4.0	308.2	309.4
o-ethyltoluene	–	11.7	1	0.5	192.2	218.6
o-fluorobenzoic acid	–	18.0	1	0.0	400.2	359.2
o-hydroxyacetanilide	21.3	24.3	1	1.0	364.5	424.2
o-hydroxybenzamide	–	21.1	1	0.0	412.2	422.0
o-hydroxybenzyl alcohol	–	15.5	1	0.5	360.2	288.9
o-hydroxybiphenyl	15.9	18.4	1	0.0	330.6	368.7
o-hydroxytoluene	15.8	14.0	1	0.0	304.2	280.7
o-methoxybenzamide	–	22.5	1	1.0	402.2	392.8
o-methoxybenzoic acid	–	21.8	1	0.5	374.2	406.0
o-methoxyphenol	–	16.9	1	0.5	305.2	314.9
o-nitroacetanilide	–	23.6	1	1.0	367.2	411.3
o-nitrobenzaldehyde	–	15.1	1	0.0	317.2	302.1
o-nitrobenzoic acid	28.0	22.0	1	0.0	419.0	440.6
o-nitrobenzyl alcohol	–	17.2	1	0.5	347.2	320.1
o-nitrophenol	17.5	15.4	1	0.0	318.2	307.7
o-nitrotoluene	–	13.8	1	0.0	269.2	275.2
o-phenylenediamine	23.1	14.0	2	0.0	373.9	315.7
o-terphenyl	17.2	19.9	1	0.5	329.4	371.0
o-toluic acid	20.2	20.0	1	0.0	376.9	400.5
o-toluidine	9.3	13.8	1	0.0	287.6	276.8
o-tolylurea	–	25.5	1	1.0	464.2	443.5
Oxasulfuron	–	44.6	1	5.5	431.2	491.9
o-xylene	13.6	11.1	2	0.0	247.8	251.3
p-acetotoluidide	–	22.3	1	1.0	427.2	387.8
p-aminobenzene sulphonamide	25.7	15.3	1	0.0	439.3	305.1
p-aminophenol	26.0	16.8	2	0.0	462.5	378.7
p-benzoquinone	18.5	16.2	4	0.0	388.0	421.0
p-bromobenzoic acid	–	21.2	2	0.0	525.2	480.2
p-bromobenzyl alcohol	–	16.4	1	0.5	350.2	305.6
p-bromophenyl urea	–	26.7	1	1.0	500.2	464.8

p-bromotoluene	15.1	12.3	2	0.0	302.2	278.9
p-chloroacetanilide	–	22.5	1	1.0	451.2	392.0
p-chloroaniline	–	14.1	2	0.0	344.2	318.1
p-chlorotoluene	13.6	11.4	2	0.0	280.7	256.6
p-cyanobenzoic acid	–	23.4	2	0.0	492.2	528.1
p-cymene	–	12.1	1	0.5	199.2	224.8
p-diethylbenzene	–	12.4	1	1.5	230.3	202.2
p-difluorobenzene	–	9.6	4	0.0	260.2	248.8
pebulate	–	29.8	1	7.5	251.2	282.8
penbutolol	–	40.2	1	6.5	343.2	410.1
pencycuron	–	41.0	1	5.5	403.2	452.0
pendimethalin	–	30.6	1	3.5	330.2	403.8
pentachlorobenzene	20.6	14.7	2	0.0	357.7	331.7
pentachloronitrobenzene	18.4	18.1	1	0.0	418.0	362.3
pentachlorophenol	17.2	18.0	2	0.0	462.5	406.9
pentaerythrityl tetrabromide	28.0	31.7	1	4.0	433.5	398.2
pentafluorochloroethane	7.6	7.1	1	0.0	173.7	142.3
pentamethylbenzene	12.9	13.5	2	0.0	328.2	304.9
pentane	8.4	12.4	1	2.0	143.5	191.0
pentanoic acid	14.2	19.7	1	2.5	239.5	287.3
pentyl 4-aminobenzoate	23.9	30.2	1	5.0	325.1	347.6
perylene	31.9	20.5	4	0.0	551.0	531.8
p-ethoxyacetanilide	31.3	28.3	1	3.0	407.2	391.8
p-ethyl hydroxybenzoate	–	21.6	1	2.0	389.2	332.8
p-ethylphenol	–	14.7	1	0.5	320.2	272.9
p-ethyltoluene	–	17.1	1	0.5	211.2	318.6
p-fluorobenzoic acid	–	19.3	2	0.0	458.2	435.2
phenanthrene	16.7	16.6	2	0.0	372.4	375.0
phenanthridine	22.9	17.4	1	0.0	379.7	347.9
phenobenzuron	–	29.6	1	3.0	392.2	410.6
phenol	11.5	13.2	2	0.0	314.0	299.3
phenolphthalein	51.1	33.5	1	0.5	534.0	624.3
phenyl glycidyl ether	17.3	21.2	1	2.0	279.8	326.4
phthalazine	13.3	12.7	2	0.0	364.5	287.1
p-hydroxybenzyl alcohol	–	18.1	1	0.5	398.2	337.1
p-hydroxytoluene	12.7	14.0	2	0.0	307.9	317.2
picric acid	17.1	21.0	1	0.0	394.1	419.2
pimilic acid	27.6	32.9	1	5.0	377.5	378.1
pirimicarb	–	22.5	1	3.0	363.7	311.2
p-isopropylbenzoic acid	–	21.0	1	0.5	391.2	390.8
p-methoxyacetanilide	27.8	25.3	1	2.0	400.3	390.9
p-methoxybenzaldehyde	–	16.8	1	0.5	275.2	313.3
p-methoxyphenol	–	17.1	1	0.5	329.2	318.5
p-methylbenzyl alcohol	–	15.2	1	0.5	333.2	282.8
p-nitroacetanilide	–	24.9	1	1.0	489.2	433.9
p-nitrobenzaldehyde	–	16.4	2	0.0	379.2	370.6
p-nitrobenzoic acid	36.9	22.7	2	0.0	512.4	512.3
p-nitrobenzyl alcohol	–	17.8	1	0.5	366.2	332.0
p-nitrophenol	18.3	16.7	2	0.0	388.2	376.9
p-N-methylhydroxyaniline	–	18.7	1	0.5	360.2	348.1

p-phenylazoaniline	21.7	19.3	2	0.0	398.2	436.4
p-phenylenediamine	21.7	16.6	4	0.0	412.3	430.2
p-propylphenol	–	17.6	1	1.5	294.2	288.2
prasterone	0.0	21.0	1	0.0	423.0	420.8
prasterone acetate	–	23.2	1	0.5	440.2	431.4
prednisolone	38.9	29.1	1	0.5	513.0	541.9
prednisone	–	30.3	1	1.0	507.2	527.1
pregnenolone	–	22.3	1	0.0	466.2	445.4
prodiamine	–	33.9	1	4.5	397.2	407.3
profluralin	–	30.3	1	3.5	306.2	398.8
progesterone	26.9	21.5	1	0.0	403.0	429.5
promecarb	–	23.9	1	3.0	360.2	330.8
prometon	–	26.1	1	2.5	365.2	380.4
prometryn	–	27.1	1	2.5	392.2	396.0
propane	3.5	5.7	2	0.0	85.5	129.4
propazine	–	28.6	1	3.5	486.2	377.3
propene	2.9	3.9	1	0.0	88.2	77.5
propoxur	–	26.5	1	4.0	360.2	332.9
propyl 4-aminobenzoate	20.5	24.3	1	3.0	347.1	336.3
propyl 4-hydroxybenzoate	28.0	24.5	1	3.0	369.2	339.6
propylcyclopentane	10.0	13.6	1	1.5	155.8	222.8
p-terphenyl	37.5	19.9	4	0.0	486.3	517.3
p-toluic acid	22.7	20.0	2	0.0	452.8	452.6
p-toluidine	17.9	13.8	2	0.0	316.5	312.8
p-xylene	17.1	11.1	4	0.0	286.3	288.8
pyrazosulfuron-ethyl	–	47.9	1	7.5	454.7	453.7
pyrene	18.4	16.9	4	0.0	423.8	440.1
pyrrole	–	14.6	2	0.0	249.8	330.7
quinoline	10.7	13.9	1	0.0	258.4	277.3
rimsulfuron	–	44.7	1	6.5	450.2	455.4
S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate	25.2	30.7	1	5.5	322.2	338.2
S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethyl phoshorodithioate	27.8	24.8	1	3.5	345.3	326.3
S-2,3,3-trichloroallyl diisopropylthiocarbamate	27.1	21.3	1	5.5	306.4	234.4
sebacic acid	40.8	41.8	1	8.0	404.0	382.4
secbumeton	–	30.7	1	5.5	361.2	338.3
sec-butylbenzene	0.0	14.2	1	1.5	204.2	233.0
siduron	–	35.6	1	5.0	409.2	409.2
simazine	–	32.0	1	3.5	498.2	421.0
simetryn	–	30.4	1	4.5	356.2	365.5
styrene	11.0	11.1	1	0.0	242.3	221.1
suberic acid	28.8	35.9	1	6.0	415.3	379.8
succinic acid	33.0	24.0	1	2.0	457.0	370.8
sulfabenzamide	–	30.7	1	2.0	454.2	473.2
sulfacetamide	–	26.8	1	1.5	456.2	438.9
sulfacytine	–	30.9	1	2.5	440.2	451.2
sulfadiazine	–	28.4	1	1.5	527.2	464.1
sulfadimethoxine	–	36.1	1	3.5	475.2	475.5
sulfaethidole	–	27.8	1	2.5	459.2	406.2
sulfamerazine	–	29.2	1	1.5	509.2	477.1

sulfameter	–	29.8	1	2.5	488.2	435.5
sulfamethazine	–	29.9	1	1.5	449.2	490.1
sulfamethizole	–	27.2	1	1.5	481.2	445.2
sulfamethomidine	–	36.1	1	2.5	419.2	526.7
sulfamethoxazole	–	26.1	1	1.5	440.2	426.6
sulfamethoxypyridazine	–	30.3	1	2.5	455.2	441.7
sulfamethylthiazole	–	28.4	1	1.5	512.2	464.2
sulfamoxole	–	27.6	1	1.5	467.2	452.5
sulfaperine	–	29.2	1	1.5	535.2	477.1
sulfapyrazine	–	28.4	1	1.5	525.2	464.1
sulfapyridine	–	27.6	1	1.5	463.2	451.0
sulfaquinoxaline	–	31.9	1	1.5	520.2	521.9
sulfathiazole	–	27.6	1	1.5	475.2	451.2
sulfisomidine	–	29.9	1	1.5	516.2	490.1
sulfisoxazole	–	26.9	1	1.5	467.2	439.6
sulfometuron-methyl	–	37.5	1	4.5	477.2	449.8
sulfosulfuron	–	48.3	1	6.5	474.6	492.8
tebuthiuron	–	28.0	1	2.0	436.2	431.5
teflubenzuron	–	33.8	1	3.0	495.7	467.5
terbumeton	–	31.1	1	3.5	396.7	410.3
terbuthylazine	–	33.7	1	2.5	451.2	492.1
terbutryn	–	32.2	1	3.5	378.2	424.4
tert-butyl bromide	10.1	11.1	3	0.0	256.1	272.6
tert-butyl chloride	11.2	10.3	3	0.0	248.1	252.5
tert-butylbenzene	8.4	12.8	1	0.0	215.0	256.0
testosterone	29.4	21.0	1	0.0	427.0	420.8
testosterone acetate	–	24.8	1	1.0	414.2	431.4
testosterone propionate	25.6	23.8	1	1.5	393.0	389.3
tetrachloroethene	11.9	8.7	4	0.0	250.8	225.3
tetradecane	45.1	39.0	1	12.0	279.0	280.8
tetrafluoroethylene	7.7	4.6	4	0.0	142.0	120.7
tetramethysuccinic acid	22.7	27.7	1	2.0	464.0	428.0
theophylline	28.2	29.0	1	0.0	544.0	579.3
thiazafluron	–	24.1	1	2.0	410.2	372.4
thiobencarb	–	26.5	1	5.0	276.5	304.4
thiofanox	–	26.8	1	4.5	330.2	321.2
thiophene	6.7	9.5	2	0.0	235.2	215.8
thymine	17.5	21.4	1	0.0	321.3	427.7
thymol	22.0	15.8	1	0.5	324.2	293.9
tolbutamide	–	33.2	1	5.5	401.2	366.4
toluene	6.6	10.3	2	0.0	178.0	233.4
trans-1,2-dimethylcyclohexane	10.5	12.7	1	3.0	185.0	175.6
trans-1,4-dimethylcyclohexane	12.3	12.7	1	3.0	236.2	175.6
trans-2-butene	9.8	5.1	2	0.0	167.6	116.2
trans-2-pentene	8.4	5.8	1	1.0	133.0	100.4
trans-azobenzene	22.5	15.8	4	0.0	341.1	410.3
triamcinolone	42.6	33.4	1	0.5	543.0	622.0
triamcinolone diacetate	–	37.6	1	3.5	508.0	495.5
triasulfuron	–	47.8	1	7.0	451.3	469.9
tribromomethane	11.1	8.9	3	0.0	281.5	217.7

trichlormethiazide	–	33.4	1	0.5	543.2	622.3
trichloroacetic acid	5.9	17.3	1	0.0	330.7	345.1
trichloroethylene	8.5	7.1	1	0.0	188.5	142.9
trichloromethane	8.8	6.4	3	0.0	209.6	157.6
tridecanoic acid	42.7	43.3	1	11.0	315.0	329.7
trietazine	–	30.0	1	3.5	374.2	395.6
triflumuron	–	37.4	1	4.0	468.2	469.7
trifluoromethane	4.1	1.0	3	0.0	118.0	24.2
trifluralin	–	30.4	1	4.5	321.7	365.1
trinitroglycerine	21.9	27.8	1	6.5	285.5	283.3
triphenylene	24.7	20.1	6	0.0	471.0	572.7
undecanedioic acid	39.7	44.7	1	9.0	385.0	383.2
undecanoic acid	34.4	37.4	1	8.5	301.6	331.4
vinyl acetate	8.5	7.9	1	1.0	180.6	137.8
vinyl chloride	4.9	4.1	1	0.0	119.3	82.2
XMC	–	22.9	1	2.0	372.2	353.7
xylylcarb	–	22.9	1	2.0	352.7	353.7
Z-3-chloro-2-butenoic acid	20.7	18.6	1	0.5	366.8	347.2

APPENDIX B. Experimental and predicted aqueous activity coefficients (γ_w) in logarithmic units for 1642 compounds.

	$\log\gamma_w$	
Name	**Exp**	**Pred**
(+)a-(3-benzoylphenyl)propionic acid	4.5	3.7
(2,4,5-trichlorophenoxy)acetic acid	2.6	3.9
(2,4-dichlorophenoxy)acetic acid	2.5	3.2
(4-chloro-2-methylphenoxy)acetic acid	3.0	3.1
(4-chloro-o-tolyloxy)acetic acid	3.0	3.1
(d) 1,2-diphenyl-1,2-dihydroxyethane	1.9	3.0
(d) 2-(m-chlorophenoxy)propanoic acid	3.0	3.0
(d) methylenebisthiopropionic acid	2.9	1.3
(Dichloromethyl)benzene	4.5	4.5
(dl) 1,2-diphenyl-1,2-dihydroxyethane	2.3	3.0
(dl) 2-(m-chlorophenoxy)propanoic acid	2.6	3.0
(dl) 2,3-dimethylpentane	6.0	4.7
(dl) 2-hexanol	2.6	3.1
(dl) 2-methyl-3-pentanol	2.4	2.8
(dl) 3,3-dimethyl-2-butanol	2.4	2.7
(dl) 3-hexanol	2.5	3.1
(dl) 3-methyl-2-butanol	1.9	2.2
(dl) 3-methylhexane	6.0	5.0
(dl) 4-methyl-2-pentanol	2.5	2.8
(dl) limonene	5.7	6.0
(dl) malathion	5.1	4.1
(dl) menthol	4.2	4.6
(dl) methylenebisthiopropionic acid	1.5	1.3
(l) menthol	4.1	4.6
1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	4.7	4.1
1-(methylamino)-9,10-anthracenedione	6.4	5.9
1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)	8.5	8.3
1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene	7.4	7.2
1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene)	7.8	8.2
1,1'-(2,2-dichloroethylidenebis(4-chlorobenzene)	7.2	7.5
1,1,1,2-Tetrachloro-2,2-difluoroethane	4.9	4.4
1,1,1,2-tetrachloroethane	3.9	4.3
1,1,1-trichloroethane	3.8	4.0
1,1,1-trifluoro-n-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide	3.9	5.5
1,1,2,2-Tetrabromoethane	4.4	4.1
1,1,2,2-tetrachlorodifluoroethane	5.0	5.0
1,1,2,2-tetrachloroethane	3.5	3.7
1,1,2-trichloroethane	3.8	3.5
1,1,2-trichlorofluoroethane	4.8	4.1
1,1,2-trichlorotrifluoroethane	4.8	4.8
1,1,2-trifluoro-1,2,2-trichloroethane	4.8	4.8
1,1,3-trimethylcyclohexane	6.6	5.8
1,1,3-trimethylcyclopentane	6.2	5.1
1,10-decanediol	2.8	4.0

1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene	7.9	7.6
1,1-dichlorobutane	4.1	4.2
1,1-dichloroethane	3.0	3.2
1,1-dichloroethylene	3.4	3.7
1,1-diethoxyethane	2.2	1.7
1,1-difluoro-1-chloroethane	3.6	3.7
1,1-dimethyl-3-phenylurea	2.3	2.4
1,1'-ethylidenebis(4-chloro-benzene)	7.5	8.2
1,2,3,4,6,7,8-heptachlorodibenzofuran	11.4	10.2
1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin	10.9	11.1
1,2,3,4,7,8-hexachlorodibenzofuran	10.6	9.6
1,2,3,4,7,8-hexachlorodibenzo-p-dioxin	9.5	10.5
1,2,3,4,7-pentachlorodibenzo-p-dioxin	9.7	9.8
1,2,3,4-tetrachlorobenzene	6.1	5.9
1,2,3,4-tetrachlorodibenzo-p-dioxin	9.3	9.2
1,2,3,4-tetrahydronaphthalene	5.2	4.8
1,2,3,4-tetrahydronaphthlene	5.2	5.1
1,2,3,5-tetrachlorobenzene	6.1	5.9
1,2,3,5-tetrafluorobenzene	4.0	4.1
1,2,3,6,7,8-hexachlorodibenzofuran	10.2	9.6
1,2,3,6,7,8-hexahydropyrene	6.6	7.0
1,2,3,7-tetrachlorodibenzo-p-dioxin	9.1	9.2
1,2,3,-trichlorobenzene	5.6	5.3
1,2,3,-trimethylbenzene	4.9	4.8
1,2,3-tribromobenzene	6.3	6.1
1,2,3-trichlorobenzene	5.4	5.3
1,2,3-trichloropropane	3.7	3.8
1,2,3-trimethylbenzene	4.9	4.8
1,2,4,5-tetrabromobenzene	7.0	7.0
1,2,4,5-tetrachloro-3-nitrobenzene	6.1	6.0
1,2,4,5-tetrachlorobenzene	6.1	5.9
1,2,4,5-tetrafluorobenzene	4.1	4.1
1,2,4,5-tetramethylbenzene	5.8	5.3
1,2,4-tribromobenzene	6.1	6.1
1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene	6.9	7.6
1,2,4-trichlorobenzene	5.4	5.3
1,2,4-trichlorodibenzo-p-dioxin	8.4	8.6
1,2,4-trimethylbenzene	5.1	4.8
1,2:3,4-dibenzanthracene	7.9	9.1
1,2:5,6-dibenzanthracene	7.7	9.1
1,2-benzacenaphthene (fluoranthene)	6.9	6.6
1,2-benzanthracene	8.0	7.7
1,2-benzofluorene	7.0	6.8
1,2-benzopyrene	8.2	8.0
1,2-bromochlorobenzene	5.4	4.9
1,2-chloronitrobenzene	4.2	4.1
1,2-dibromo-3-chlorpropane	4.1	4.1
1,2-dibromobenzene	5.2	5.2
1,2-dibromoethane	3.4	3.5
1,2-dibromoethylene	3.1	4.0

1,2-dibromopropane	3.9	3.7
1,2-dibromotetrafluoroethane	6.7	5.0
1,2-dicarbomethoxybenzene	3.4	3.5
1,2-dichlorobenzene	5.0	4.7
1,2-dichloroethane	3.0	3.3
1,2-dichloroethylene	3.0	3.5
1,2-dichloropropane	3.3	3.5
1,2-dichlorotetrafluoroethane	4.5	4.7
1,2-dichloro-tetrafluoroethane	4.9	4.7
1,2-dicyanobenzene	3.3	3.0
1,2-diethoxyethane	1.9	2.0
1,2-diethylbenzene	5.0	5.4
1,2-difluorobenzene	2.7	3.7
1,2-diiodobenzene	6.0	5.9
1,2-diiodoethylene	5.0	4.7
1,2-dinitrobenzene	3.3	3.6
1,2-diphenylethane	6.0	6.1
1,2-propylene oxide	2.3	1.7
1,3,5-tribromobenzene	5.8	6.1
1,3,5-trichlorobenzene	5.2	5.3
1,3,5-trimethylbenzene	5.1	4.8
1,3,5-trinitro-1,3,5-triazacyclohexane	2.8	2.4
1,3,5-trinitrobenzene	4.0	3.8
1,3,6,8-tetrachlorodibenzo-p-dioxin	9.2	9.2
1,3-bromochlorobenzene	5.0	4.9
1,3-butadiene	3.6	3.1
1,3-dibromobenzene	5.3	5.2
1,3-dibromopropane	3.8	4.1
1,3-dicarbomethoxybenzene	4.0	3.5
1,3-dichloro-2-propanol	1.9	2.1
1,3-dichlorobenzene	4.8	4.7
1,3-dichloropropane	3.4	3.8
1,3-difluorobenzene	3.7	3.7
1,3-diiodobenzene	6.2	5.9
1,3-dimethylnaphthalene	6.0	5.8
1,3-dinitrobenzene	3.7	3.6
1,3-diphenylurea	2.4	3.2
1,3-nitrochlorobenzene	4.3	4.1
1,4,5-trimethylnaphthalene	6.3	6.3
1,4-bromochlorobenzene	5.0	4.9
1,4-bromoiodobenzene	5.7	5.5
1,4-cyclohexadiene	3.8	3.9
1,4-diamino-2-methoxyanthraquinone	4.9	4.6
1,4-diaminoanthraquinone	6.0	4.5
1,4-dibromobenzene	5.1	5.2
1,4-dicarbomethoxybenzene	4.2	3.5
1,4-dichloro-2,5-dimethoxybenzene	4.9	4.9
1,4-dichlorobenzene	4.7	4.7
1,4-diethylbenzene	5.5	5.4
1,4-difluorobenzene	3.7	3.7

1,4-dihydroxybenzene	0.3	0.6
1,4-diiodobenzene	6.1	5.9
1,4-dimethylnaphthalene	5.9	5.8
1,4-dinitrobenzene	3.5	3.6
1,4-nitrochlorobenzene	4.3	4.1
1,4-pentadiene	3.8	4.2
1,5-dichloro-3-oxapentane	2.7	3.0
1,5-dimethylnaphthalene	6.0	5.8
1,5-hexadiene	4.4	4.4
1,8-dimethylnaphthalene	6.2	5.8
10H-phenothiazine	5.2	5.5
11-alpha-hydroxyprogesterone	4.3	4.4
13H-dibenzo(a,i)carbazole	7.7	7.9
17-methyltestosterone	4.5	5.2
1a,2a,3ß,4a,5a,6ß-hexachlorocyclohexane	5.4	6.4
1-aminoanthraquinone	5.4	5.0
1-anthranol	5.4	4.9
1-bromo-2-chlorobenzene	4.9	4.9
1-bromo-2-chloroethane	3.1	3.4
1-bromo-2-ethylbenzene	5.4	5.3
1-bromo-2-methylpropane	4.2	3.8
1-bromo-3-chloropropane	3.6	3.9
1-bromo-3-methylbutane	4.6	4.4
1-bromo-4-chlorobenzene	4.9	4.9
1-bromobutane	3.9	4.2
1-bromoheptane	6.2	5.7
1-bromohexane	5.5	5.2
1-bromonaphthalene	6.1	5.7
1-bromooctane	6.8	6.3
1-bromooctane	6.8	6.3
1-bromopentane	4.8	4.7
1-bromopropane	3.4	3.6
1-butene	4.1	3.5
1-butyne	3.0	3.0
1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene	7.8	8.3
1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene	7.5	7.6
1-chloro-2-bromoethane	3.1	3.4
1-chloro-2-methylpropane	3.7	3.7
1-chlorobutane	3.7	4.0
1-chlorodibenzodioxin	6.6	7.1
1-chlorodibenzo-p-dioxin	6.8	7.3
1-chloroheptane	5.7	5.6
1-chlorohexane	4.9	5.1
1-chloronaphthalene	5.7	5.5
1-chloropentane	4.5	4.6
1-chloropropane	3.2	3.5
1-decanol	5.4	5.4
1-decene	7.1	6.7
1-ethylnaphthalene	5.9	5.8
1-ethyltheobromine	1.1	2.1

1-fluoro-4-iodobenzene	4.9	4.9
1-heptanethiol	5.9	5.4
1-heptanol	3.5	3.9
1-heptene	5.5	5.1
1-heptyne	4.8	4.6
1-hexanol	3.0	3.3
1-hexen-3-one	2.6	2.5
1-hexene	5.0	4.6
1-hexene-3-ol	2.3	3.0
1-hexyne	3.9	4.1
1-hydroxychlordene	5.7	4.5
1-iodobutane	4.7	4.6
1-iodoheptane	6.6	6.2
1-iodonaphthalene	6.3	6.1
1-iodopropane	3.9	4.1
1-methyl fluorene	6.4	6.2
1-methyl-1-cyclohexene	5.0	4.4
1-methylcyclohexene	5.0	4.4
1-methylnaphthalene	5.5	5.3
1-methylphenanthrene	6.7	6.7
1-naphthaleneacetamide	3.4	3.7
1-naphthaleneacetic acid	3.4	4.1
1-naphthoic acid	3.9	3.6
1-naphthyl methylcarbamate	3.8	4.1
1-naphthylamine	3.5	4.1
1-nitronaphthalene	5.7	5.0
1-nonanol	4.8	4.9
1-nonene	6.8	6.2
1-nonyne	6.0	5.7
1-octanol	4.1	4.4
1-octene	6.2	5.6
1-octyne	5.4	5.1
1-pentadecanol	7.5	8.1
1-pentanethiol	4.6	4.4
1-pentanol	2.3	2.8
1-pentene	4.4	4.1
1-pentyne	3.4	3.6
1-phenylethanol	2.7	2.8
1-propanethiol	3.3	3.3
1-propyl nitrate	3.2	3.5
1-tetradecanol	7.4	7.5
2-(1,3-dioxolan-2-yl)phenyl methylcarbamate	2.3	2.9
2-(1'-cyclohexenyl)cyclohexanone	4.5	5.2
2-(1-methylethyl)phenyl methylcarbamate	3.5	4.0
2-(2,4,5-trichlorophenoxy)propanoic acid	2.5	4.2
2-(2,4-dichlorophenoxy)propanoic acid	3.3	3.6
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	5.7	4.7
2-(4-chloro-2-methylphenoxy)propanoic acid	3.3	3.4
2-(6-methoxy-2-naphthyl)propionic acid	4.2	4.0
2,2,2,o,p'-pentachloroethylidenebisbenzene	8.0	8.3

2,2',3,3',4,4',5,5' 6'-nonachlorodiphenyl ether	11.0	11.2
2,2',3,3',4,4',5,5',6-nonachlorobiphenyl	10.4	11.0
2,2',3,3',4,4',5,5'-octachlorobiphenyl	10.1	10.4
2,2',3,3',4,4',5,5'-octachlorodiphenyl ether	11.0	10.0
2,2',3,3',4,4',5-heptachlorodiphenyl ether	10.1	9.9
2,2',3,3',4,4',6-heptachlorobiphenyl	9.2	9.8
2,2',3,3',4,4'-hexachlorobiphenyl	8.4	9.1
2,2',3,3',4,4'-hexachlorodiphenyl ether	8.7	9.3
2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	10.8	11.0
2,2',3,3',4,5,5'6'-octachlorodiphenyl ether	10.0	10.6
2,2',3,3',4',5,6-heptachlorodiphenyl ether	10.3	9.9
2,2',3,3',4,5-hexachlorobiphenyl	8.9	9.1
2,2',3,3',4-pentachlorobiphenyl	8.0	8.5
2,2',3,3',5,5',6,6'-octachlorobiphenyl	10.0	10.4
2,2',3,3',5,5',6-heptachlorobiphenyl	9.5	9.8
2,2',3,3',5,5'-hexachlorobiphenyl	8.4	9.1
2,2',3,3',5',6-hexachlorobiphenyl	8.7	9.1
2,2',3,3',6,6'-hexachlorobiphenyl	8.8	9.1
2,2',3,3'-tetrachlorobiphenyl	8.2	7.9
2,2',3,4,4',5,5'6-octachlorodiphenyl ether	10.4	10.6
2,2',3,4,4',5,5'-heptachlorodiphenyl ether	10.6	9.9
2,2',3,4,4',5',6-heptachlorobiphenyl	9.2	9.8
2,2',3,4,4',5'-hexachlorobiphenyl	8.9	9.1
2,2',3',4,4',5-hexachlorodiphenyl ether	9.6	9.3
2,2',3,4,4',5'-hexachlorodiphenyl ether	9.6	9.3
2,2',3,4,4',6'-hexachlorodiphenyl ether	8.9	8.8
2,2',3,4,4'-pentachlorodiphenyl ether	8.8	8.7
2,2',3,4,5,5',6-heptachlorobiphenyl	9.6	9.8
2,2',3,4',5,5',6-heptachlorobiphenyl	9.6	9.8
2,2',3,4',5,5',6-heptachlorodiphenyl ether	9.9	9.9
2,2',3,4,5,5'-hexachlorobiphenyl	8.9	9.1
2,2',3,4,5'-pentachlorobiphenyl	7.9	8.5
2,2',3,4,5-pentachlorobiphenyl	8.3	8.5
2,2',3,4,6-pentachlorobiphenyl	8.5	8.5
2,2',3,5,5',6-hexachlorobiphenyl	8.5	9.1
2,2',3,5'-tetrachlorobiphenyl	8.0	7.9
2,2,3-trimethyl-3-pentanol	3.0	3.6
2,2',4,4',5,5'-hexachlorobiphenyl	8.8	9.1
2,2',4,4',5,5'-hexachlorodiphenyl ether	9.2	9.3
2,2',4,4',5,6'-hexachlorodiphenyl ether	9.1	8.8
2,2',4,4',6,6'-hexachlorobiphenyl	10.0	9.1
2,2',4,4'-tetrachlorobiphenyl	7.7	7.9
2,2',4,4'-tetrachlorodiphenyl ether	8.1	8.0
2,2',4,5,5'-pentachlorobiphenyl	8.6	8.5
2,2',4',5-tetrachlorobiphenyl	8.5	7.9
2,2',4,5'-tetrachlorobiphenyl	8.0	7.9
2,2',4,6,6'-pentachlorobiphenyl	8.5	8.5
2,2,4-trimethylpentane	6.4	5.1
2,2',5,5'-tetrabromobiphenyl	9.0	8.9
2,2',5,5'-tetrachlorobiphenyl	7.5	7.9

2,2',5,6'-tetrachlorobiphenyl	7.9	7.9
2,2',5-trichlorobiphenyl	7.2	7.2
2,2,5-trimethylhexane	6.8	5.6
2,2',6,6'-tetrachlorobiphenyl	7.6	7.9
2,2'-dichlorobiphenyl	6.7	6.6
2,2-dimethyl-1-butanol	2.8	2.9
2,2-dimethyl-1-pentanol	3.3	3.4
2,2-dimethyl-1-propanol	2.1	2.4
2,2-dimethyl-3-pentanol	2.9	3.2
2,2-dimethylbutane	5.4	4.4
2,2-dimethylpentane	6.1	4.9
2,2-dimethylpropane	5.1	3.8
2,2-dimethylpropanoic acid (pivalic acid)	2.3	1.8
2,3,3',4,4',5-hexachlorobiphenyl	8.6	9.1
2,3,3',4,4',5-hexachlorodiphenyl ether	9.4	9.3
2,3,3',4,4',6-hexachlorobiphenyl	8.7	9.1
2,3,3',4,4'-pentachlorodiphenyl ether	9.0	8.7
2,3,3',4',5,6-hexachlorobiphenyl	8.7	9.1
2,3,3'4,4',5,6-heptachlorodiphenyl ether	9.8	9.9
2,3,3-trimethyl-2-butanol	2.5	3.1
2,3',4,4',5,5'-hexachlorodiphenyl ether	9.9	9.3
2,3,4,4',5,6-hexachlorodiphenyl ether	9.5	9.3
2,3',4,4',5-pentachlorobiphenyl	8.4	8.5
2,3',4,4'-tetrachlorobiphenyl	7.7	7.9
2,3,4,5,6-pentachlorobiphenyl	8.7	8.5
2,3,4,5-tetrachloroanisole	6.4	6.0
2,3,4,5-tetrachlorobiphenyl	8.3	7.9
2,3',4',5-tetrachlorobiphenyl	8.3	7.9
2,3,4,7,8-pentachlorodibenzofuran	9.4	8.9
2,3,4-trichloroanisole	5.6	5.4
2',3,4-trichlorobiphenyl	7.7	7.2
2,3,4'-trichlorobiphenyl	7.6	7.2
2,3,4-trimethylpentane	6.4	4.9
2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione	2.2	4.1
2,3',5-trichlorobiphenyl	7.6	7.2
2,3,6-trichlorobiphenyl	7.8	7.2
2,3,6-trichlorophenylacetic acid	3.6	4.5
2,3,7,8-tetrachlorodibenzofuran	9.0	8.3
2,3,7,8-tetrachlorodibenzo-p-dioxin	9.8	8.6
2,3-benzofluorene	8.2	6.8
2,3-benzofluorene	7.9	6.9
2,3-dichloro-1,4-naphthalenedione	6.3	5.3
2,3-dichloro-2-methylbutane	4.4	4.1
2,3-dichloroanisole	5.0	4.8
2,3-dichlorobutane	4.1	3.7
2,3-dichlorodibenzo-p-dioxin	7.9	8.0
2,3-dichlorophenol	3.0	3.1
2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	3.0	3.8
2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	2.8	3.0
2,3-dimethyl-1,3-butadiene	4.1	4.6

2,3-dimethyl-1-butanol	2.1	2.6
2,3-dimethyl-2-butanol	2.1	2.7
2,3-dimethyl-3-pentanol	2.6	3.2
2,3-dimethylbutane	5.3	4.1
2,3-dimethylbutanol	2.1	2.7
2,3-dimethylnaphthalene	6.0	5.8
2,3-dimethylphenol	2.7	3.0
2,3-dinitrotoluene	4.3	4.1
2,4,4',6-tetrachlorobiphenyl	8.2	7.9
2,4,4'-trichlorobiphenyl	7.7	7.2
2,4,4'-trichlorodiphenyl ether	7.7	7.4
2,4,5,6-tetrachloro-1,3-benzenedicarbonitile	5.1	5.5
2,4,5,6-tetrachloroanisole	6.5	6.0
2,4,5-trichlorobiphenyl	7.4	7.2
2,4',5-trichlorobiphenyl	7.6	7.2
2,4,5-trichlorodiphenyl ether	8.0	7.4
2,4,5-trichlorophenol	3.5	3.7
2,4,6-N-tetranitroethylaniline	4.6	5.2
2,4,6-tribromobiphenyl	8.7	8.0
2,4,6-tribromophenol	4.8	4.3
2,4,6-trichloroanisole	5.6	5.4
2,4,6-trichlorobiphenyl	7.4	7.2
2,4,6-trimethyl-1,3,5-trioxane	1.8	3.1
2,4,6-trimethylpyridine	2.3	4.0
2,4,6-trinitroresorcinol	1.4	2.0
2,4,6-trinitrotoluene	4.4	4.2
2,4,6-tri-tert-butylphenol	4.7	6.9
2,4-dibromophenol	3.7	3.6
2,4'-dichlorobiphenyl	6.9	6.6
2,4-dichlorobiphenyl	7.0	6.6
2,4'-dichlorodiphenyl ether	7.2	6.8
2,4-dichlorophenol	3.1	3.1
2,4-dichlorophenyl 4-nitrophenyl ether	6.7	6.9
2,4-dimethyl-1-pentanol	3.3	3.2
2,4-dimethyl-2-pentanol	2.7	3.2
2,4-dimethyl-3-pentanol	3.0	3.0
2,4-dimethylpentane	6.0	4.7
2,4-dimethylphenol	2.9	3.0
2,4-dinitrochlorobenzene	5.8	4.3
2,4-dinitrophenol	2.6	2.5
2,4-dinitrotoluene	4.1	4.1
2,4-octadione	3.3	2.8
2,5-dichlorobiphenyl	7.0	6.6
2,5-dichlorophenol	3.3	3.1
2,5-dimethoxybenzaldehyde	3.8	3.5
2,5-dimethylaniline	3.1	3.6
2,5-dimethylphenol	2.7	3.0
2,5-dinitrophenol	3.5	2.5
2,6-dichloro-4-benzenamine	2.2	3.9
2,6-dichloro-4-nitroaniline	4.1	3.6

2,6-dichloroanisole	4.8	4.8
2,6-dichlorobenzonitrile	4.3	4.5
2,6-dichlorobenzyl alcohol	3.2	3.7
2,6-dichlorobiphenyl	6.6	6.6
2,6-dichlorodiphenyl ether	6.7	6.8
2,6-dichlorophenol	3.2	2.9
2,6-dimethylnaphthalene	5.7	5.8
2,6-dimethylphenol	2.8	3.0
2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	7.7	7.6
2,6-di-tert-butyl-4-methylphenol	6.7	5.7
2,6-di-tert-butylphenol	6.5	5.2
2,7-dichlorodibenzo-p-dioxin	8.2	8.0
2,7-dimethylnaphthalene	5.8	5.8
2,8-dichlorodibenzofuran	7.6	7.0
2,8-dichlorodibenzo-p-dioxin	7.8	8.0
2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	5.1	5.0
2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	3.4	4.5
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	2.5	3.0
2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	0.2	-0.4
2-aminobenzoic acid	2.3	1.9
2-bromo-2-chloro-1,1,1-trifluoroethane	3.4	4.2
2-bromofluorobenzene	4.4	4.5
2-bromonaphthalene	5.8	5.7
2-bromonaphthalene	5.8	5.7
2-bromopropane	3.3	3.3
2-bromotoluene	4.0	4.8
2-butanethiol	3.6	3.5
2-butoxyethanol	2.2	2.0
2-butyl benzene	5.6	5.3
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	7.3	8.3
2-chloro-2-methylbutane	4.3	4.1
2-chloro-6-(trichloromethyl)pyridine	4.8	5.0
2-chloroanisole	4.2	4.1
2-chlorobenzoic acid	2.4	3.1
2-chlorobiphenyl	6.3	6.0
2-chlorobutane	3.7	3.7
2-chlorodibenzodioxin	6.9	7.1
2-chlorodibenzo-p-dioxin	7.0	7.3
2-chlorodiphenyl ether	6.3	6.2
2-chloro-n-(2,6-diethylphenyl)-n-(methoxymethyl)acetamide	4.5	3.6
2-chloronaphthalene	5.6	5.5
2-chloro-N-isopropyl N-phenylacetamide	3.5	3.2
2-chloropentane	4.1	4.2
2-chlorophenol	2.4	2.4
2-chloropropane	3.1	3.2
2-cyclohexyl-4,6-dinitrophenol	4.9	5.1
2-decanone	5.0	5.2
2-ethyl-1,3-hexanediol	2.3	2.4
2-ethyl-1-butanol	2.9	3.0
2-ethyl-1-hexanol	3.9	4.1

2-ethyl-2-propanol	1.9	2.4
2-ethylanthracene	7.5	7.3
2-ethylnaphthalene	6.0	5.8
2-ethylphenol	3.1	3.0
2-ethylthiophene	4.3	3.7
2-ethyltoluene	5.0	4.9
2-heptanol	3.3	3.6
2-heptanone	3.2	3.6
2-hexanone	2.5	3.1
2-hexanone	2.5	3.1
2-hydroxybenzoic acid	2.2	1.3
2-imidazolidinethione	0.9	0.5
2-iodobenzoic acid	3.3	3.7
2-iodopropane	3.8	3.8
2-isopropoxyphenyl N-methylcarbamate	3.1	3.5
2-isopropyltoluene	5.5	5.2
2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide	5.0	4.2
2-methoxypteridine	1.7	1.8
2-methyl pentane	5.5	4.4
2-methyl-1,3-butadiene	3.8	3.9
2-methyl-1-butanol	2.2	2.5
2-methyl-1-butene	4.5	3.9
2-methyl-1-pentanol	2.8	3.0
2-methyl-1-pentene	4.8	4.4
2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime	2.4	2.4
2-methyl-2-butene	4.3	3.5
2-methyl-2-heptanol	3.5	4.0
2-methyl-2-hexanol	2.8	3.5
2-methyl-2-pentanol	2.2	3.0
2-methyl-3-pentanol	2.4	2.7
2-methyl-4,6-dinitrophenol	4.2	3.0
2-methylanthracene	6.9	6.7
2-methylbutane	4.9	3.6
2-methylcyclohexanone	2.7	3.2
2-methylfuran	3.2	3.4
2-methylheptane	6.2	5.5
2-methylhexane	6.3	5.0
2-methylnaphthalene	5.4	5.3
2-methylpentane	5.5	4.4
2-methylphenanthrene	7.3	6.7
2-methylpropane	4.3	3.4
2-methylpropene	4.1	3.4
2-naphthoic acid	3.9	3.6
2-naphthylamine	5.2	4.1
2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	6.4	7.1
2-nitro-5-methylphenol	4.4	2.9
2-nitroaniline	3.3	3.0
2-nonanol	4.5	4.7
2-nonanone	4.3	4.7
2-octanol	3.8	4.1

2-octanone	3.9	4.1
2-pentanol	2.0	2.6
2-pentanol	2.0	2.6
2-pentanone	1.9	2.6
2-pentanone	2.0	2.6
2-pentene	4.3	3.7
2-phenoxyethanol	2.4	2.6
2-phenyl-3,1-benzoxazin-4-one	5.5	5.1
2-phenylethanol	2.5	2.9
2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate	6.8	6.3
2-undecanol	4.7	5.7
3-(3,4-dichlorophenyl)-1,1-dimethylurea	3.7	3.7
3-(4-chlorophenyl)-1,1-dimethylurea	3.0	3.1
3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	2.4	2.7
3(n-octyloxy)-1,2-propanediol	3.7	2.9
3-(p-tolyl-4-sulfonyl)-1-butyl urea	4.0	3.9
3,3',4,4'-tetrachlorobiphenyl	9.1	7.9
3,3',4,4'-tetrachlorodiphenyl ether	8.3	8.0
3,3',5,5'-tetrachlorobiphenyl	9.3	7.9
3,3'-dichlorobiphenyl	7.5	6.6
3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime	3.0	3.2
3,3-dimethyl-1-butanol	2.2	2.9
3,3-dimethyl-2-butanol	2.4	2.6
3,3-dimethyl-2-butanone	2.5	2.7
3,3-dimethylpentane	6.0	4.9
3,3'-di-tert-butyl-5,5'-dimethyl-2,2-dihydroxydiphenylmethane	7.6	7.3
3,4,4'-trichlorobiphenyl	8.2	7.2
3,4,5,6-tetrachloroveratrole	6.3	6.1
3,4,5-trichlorodiphenyl ether	8.2	7.4
3,4,5-trichloroveratrole	5.7	5.5
3,4-benzophenanthrene	9.5	7.7
3,4-benzopyrene	8.3	8.0
3,4-dichloro-2-methoxybenzoic acid	1.4	3.6
3,4-dichlorobiphenyl	9.0	6.6
3,4-dichloronitrobenzene	4.8	4.8
3,4-dichlorophenol	2.5	3.3
3',4'-dichloropropionanilide	4.3	3.9
3,4-dimethylisoxazol 5-sulphanylamide	3.0	3.0
3,4-dimethylphenol	2.8	3.0
3,4-dimethylphenyl methylcarbamate	3.7	3.6
3,4-dinitrotoluene	4.7	4.1
3,5,6-trichloro-2-pyridinyloxyacetic acid	2.9	3.1
3,5-dibromo-4-hydroxybenzonitrile	3.1	3.2
3,5-dichlorobenzoic acid	3.4	3.4
3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	4.4	4.1
3,5-dichlorophenol	2.8	3.3
3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate	4.5	4.1
3,5-dimethylphenol	2.8	3.0
3,5-dimethylphenyl methylcarbamate	3.5	3.6
3,5-dinitrobenzoic acid	2.4	2.4

3,6-dichloro-2-methoxybenzoic acid	2.2	3.6
3-amino-2,5-dichlorobenzoic acid	1.8	2.8
3-aminobenzoic acid	1.8	1.4
3-bromo-4-hydroxybenzaldehyde	3.1	2.8
3-bromopropylene	3.2	3.0
3-chloroanisole	4.5	4.1
3-chlorobenzoic acid	3.0	2.8
3-chlorobiphenyl	6.5	6.0
3-chloropentane	4.4	4.2
3-chlorophenol	2.4	2.6
3-chloropropionitrile	2.0	2.4
3-chloropropylene	3.1	3.3
3-ethoxy-4-hydroxybenzaldehyde	2.9	2.5
3-ethyl-3-pentanol	2.6	3.5
3-heptanol	3.2	3.6
3-heptanone	3.2	3.6
3-hexanol	2.5	3.1
3-hexanone	2.6	3.1
3-hexyne	3.7	3.9
3-hydroxybenzoic acid	1.3	0.8
3-hydroxytoluene	2.4	2.5
3-iodobenzoic acid	3.2	3.4
3-methyl cholanthrene	8.3	8.6
3-methyl-1-butanol	2.3	2.5
3-methyl-1-butanol acetate	3.7	3.4
3-methyl-1-butene	4.5	3.9
3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	3.5	3.8
3-methyl-2-butanol	1.9	2.2
3-methyl-2-butanone	1.9	2.4
3-methyl-2-heptanol	3.5	3.8
3-methyl-2-pentanol	2.5	2.7
3-methyl-2-pentanone	2.4	2.9
3-methyl-3-heptanol	3.3	4.0
3-methyl-3-hexanol	2.7	3.5
3-methyl-3-pentanol	2.1	3.0
3-methylacetanilide	3.4	2.6
3-methylcyclohexanone	3.6	3.2
3-methylheptane	6.9	5.5
3-methylindole	3.5	4.1
3-methylpentane	5.4	4.4
3-methylthiophene	4.1	3.2
3-nitroaniline	2.8	2.7
3-nitrotoluene	4.2	4.0
3-octanol	3.7	4.1
3-pentanol	2.0	2.6
3-pentanone	2.0	2.6
3-pentenenitrile	2.7	2.9
3-phenyl-1-propanol	3.1	3.5
3-phenylpropanol	3.1	3.5
3-propyl-2,4-pentadione	2.6	2.6

4-(1,1-dimethylethyl)-n-(1-methylpropyl)-2,6-dinitrobenzeneamine	6.8	7.2
4-(2,4,5-trichlorophenoxy)butanoic acid	4.4	4.9
4-(2,4-dichlorophenoxy)butyric acid	3.9	4.3
4-(4-chloro-2-methylphenoxy)butanoic acid	4.3	4.1
4-(4-chloro-2-methylphenoxy)butanoic acid	4.3	4.1
4-(4-nitrophenylazo)aniline	5.4	5.0
4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide	5.0	5.1
4,4'-dibromobiphenyl	8.5	7.1
4,4'-dichlorobiphenyl	7.2	6.6
4,4'dihydroxydiphenyl-2,2-propane	3.4	4.3
4,4-dimethyl-1-pentanol	3.3	3.4
4,5-dichloroquiaiacol	3.8	3.4
4,5-dichloroveratrole	4.6	4.9
4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	4.6	3.9
4-aminoacetophenone	1.9	2.0
4-aminobenzoic acid	1.8	1.4
4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide	3.7	2.5
4-aminopyridine	0.7	1.8
4-bromophenol	2.5	2.9
4-bromotoluene	4.9	4.8
4-chloroanisole	4.5	4.1
4-chloroazobenzene	6.6	6.3
4-chlorobenzoic acid	2.7	2.8
4-chlorobiphenyl	6.5	6.0
4-chlorophenol	2.3	2.6
4-chlorophenoxyacetic acid	2.1	2.6
4-ethoxy-3-methoxybenzaldehyde	3.4	4.0
4-ethyltoluene	4.9	4.9
4-heptanol	3.1	3.6
4-heptanone	3.3	3.6
4-hexylresorcinol	3.9	3.7
4-hydroxy-3,5-diiodobenzonitrile	3.4	3.9
4-hydroxyazobenzene	3.4	4.3
4-hydroxybenzoic acid	1.1	0.8
4-hydroxyphenylacetic acid	1.2	1.2
4-iodoacetanilide	3.4	3.4
4-iodobenzoic acid	2.9	3.4
4-isopropyltoluene	5.5	5.2
4-methoxybenzoic acid	2.5	2.3
4-methoxyphenol	1.9	2.1
4-methoxyphenylpropionic acid	2.9	3.0
4-methoxypteridine	1.3	1.8
4-methyl-1-pentanol	2.9	3.0
4-methyl-1-pentene	5.0	4.3
4-methyl-2-pentanol	2.5	2.8
4-methyl-2-pentanone	2.5	2.8
4-methylbiphenyl	6.2	5.8
4-methylcyclohexanol	2.6	3.2
4-methyloctane	7.8	6.0
4-methylpent-1-ene	5.0	4.3

4-methylphenanthrene	7.4	6.7
4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline	6.0	6.1
4-methylthio-3,5-xylyl methylcarbamate	4.4	4.4
4-methyoxyacetanilide	1.8	2.3
4-nitro-5-methylphenol	2.6	2.6
4-nitroaniline	2.9	2.7
4-nitrotoluene	4.0	4.0
4-oxaheptane	3.1	3.4
4-pentene-1-ol	1.9	2.6
4-tert-butylbenzoic acid	4.5	3.8
4-tert-butylphenol	3.6	3.6
5'-(trifluoromethanesulphonamide)acet-2',4-xylidide	2.7	3.1
5,6-dehydroisoandrosterone acetate	4.8	5.4
5,6-dimethylchrysene	7.8	6.8
5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione	3.1	2.9
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	3.5	2.7
5-ethylhydantoin	0.9	0.4
5-isopropyl-2-methylphenol (carvacrol)	3.8	3.8
5-isopropyl-m-tolyl methylcarbamate	4.4	4.5
5-methyl N-(methylcarbamoyloxy)thioacetimidate	1.6	1.5
5-methyl-1,2,4-triazolo[3,4-b]benzothiazole	2.3	4.3
5-methyl-2-hexanol	3.1	3.3
5-methyl-2-hexanone	3.1	3.3
5-methylchrysene	7.5	8.2
5-nonanone	4.3	4.7
6-methyl-2,4-heptadione	3.3	2.4
6-methylchrysene	7.1	8.2
7,8-benzoquinoline	4.9	5.5
8-quinolinol	3.7	2.7
9,10-dimethyl-1,2-benzanthracene	7.7	8.7
9,10-dimethylanthracene	7.2	7.2
9-methylanthracene	7.2	6.7
acenaphthalene	5.2	5.3
acenaphthene	5.6	5.3
acenaphthylene	5.2	5.3
acetanilide	2.2	2.1
acetohexamide	1.0	3.0
acetophenone	3.0	2.7
acetylene	3.1	2.2
acridine	4.7	5.5
adenine	1.2	0.5
adipic acid	0.6	0.6
adrenosterone	3.8	2.5
a-endosulfan	6.9	6.3
alachlor	4.7	4.8
Aldicarb	2.2	2.4
aldosterone	4.1	1.5
Aldoxycarb	1.5	1.2
aldrin	7.4	7.6
allobarbitiol	2.0	1.7

allopurinol	1.1	-0.2
allyl bromide	3.2	3.5
allyl chloride	3.1	3.3
alpha-chlorotoluene	4.1	4.2
alpha-estradiol	5.1	4.6
alpha-Pinene	6.5	4.8
amertryn	3.9	3.3
a-methylstyrene	4.9	5.1
ametryn	4.0	4.0
aminocarb	3.2	3.6
amobarbital	2.4	2.3
amylacetate	3.6	3.7
a-naphthol	3.2	3.4
a-naphthyl acetate	4.2	4.1
androstane-17-one	6.6	6.4
androstanedione	4.5	5.1
androstanolone	4.3	5.2
androsterone	4.7	5.2
anethole	4.9	5.0
aniline	2.2	2.6
anisole	3.6	3.5
anthracene	6.3	6.3
anthraquinone	4.3	5.5
aprobarbital	2.0	1.9
atrazine	3.5	3.7
atropine	2.6	2.6
azelaic acid	2.4	2.2
b(4-chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	4.5	4.3
barban	5.4	4.4
barbital	1.6	1.0
benazolin	2.7	1.4
bendiocarb	3.5	3.3
bendroflumethiazide	3.3	3.3
benfluralin	7.7	7.6
benodanil	4.7	4.6
bensulide	5.8	6.4
benzaldehyde	2.9	3.3
benzaldehyde	2.9	3.3
benzamide	1.9	2.3
benzamide	1.9	2.3
benzene	3.4	3.4
benzhydrol	3.9	3.8
benzidine	3.6	3.8
benzimidazole	2.4	2.8
benzo(a)fluorene	7.0	6.9
benzo(b)fluoranthene	8.3	8.0
benzo(e)pyrene	8.4	8.0
benzo(g,h,i)perylene	8.8	8.3
benzo(j)fluoranthene	8.5	8.0
benzo(k)fluoranthene	8.7	8.0

benzofluoranthene	9.0	6.8
benzoic acid	2.5	2.2
benzoin	3.4	3.2
benzonitrile	3.5	3.2
benzophenone	4.6	4.6
benzothiazole	3.2	3.4
benzothiophene	4.7	4.2
benzotrifluoride	4.8	4.8
benzoxazole	2.9	3.6
benzyl alcohol	2.1	2.4
benzyl alcohol	2.1	2.4
benzyl butyl phthalate	7.4	6.8
benzyl chloride	4.1	4.2
benzylurea	1.3	1.3
beta-endosulfan	6.2	7.6
betamethasone	3.6	2.8
betamethasone-17-valerate	4.0	5.2
beta-naphthol	3.2	3.4
bibenzyl	6.1	6.1
biphenyl	5.7	5.4
bis-(2-chloroethyl)-ether	2.9	3.0
bis-(2-chloroethyl)-sulfone	2.8	3.1
bis-(2-chloroethyl)-sulfoxide	1.8	1.7
bis-(4-aminophenyl)methane	3.7	4.4
borneol(sp)	2.5	3.7
bromazepam	3.4	2.9
bromobenzene	4.3	4.3
bromochloromethane	2.6	3.1
bromocyclohexane	4.0	4.4
Bromodichloromethane	3.5	3.1
bromoethane	2.8	3.1
bromomethane	2.5	2.6
bromophos	7.5	6.8
bromopropylate	6.0	6.3
Butacarb	5.1	5.9
butachlor	5.9	5.2
butalbital	2.3	2.4
butamben	4.4	4.3
butanal	1.7	2.0
butane	4.7	3.7
butanethiol	3.9	3.8
butanoic acid	1.9	1.7
butethal	2.2	3.0
butocarboxim	2.5	2.4
buturon	4.1	3.8
butyl 4-aminobenzoate	4.1	4.3
butyl 9-hydroxy-9H-fluorene-9-carboxylate	5.0	4.6
butyl acetate	3.0	3.2
butyl acrylate	3.5	3.8
butyl alcohol	1.8	2.3

butyl benzene	5.8	5.4
Butyl benzyl phthalate	6.8	6.8
butyl butanoate	4.2	4.2
butyl ethanoate	2.9	3.2
butylate	5.4	5.5
butyltoluene	5.8	5.9
butyraldehyde	1.8	2.0
caffeine	0.9	0.5
camphor(sp)	2.4	3.7
caproaldehyde	3.0	3.1
caprylaldehyde	4.1	4.1
carbaryl	3.6	4.1
carbazole	4.7	5.0
carbendazim	3.0	2.1
carbofuran	3.1	4.2
carbon tetrabromide	4.5	5.0
carbon tetrachloride	4.0	4.5
carbon tetrafluoride	5.4	4.0
carbophenothion	7.5	7.4
carboxin	4.2	3.9
carbutamide	2.6	2.4
carvone	3.8	4.7
chloralose	1.6	-0.1
chloramben methyl ester	4.7	3.9
chloramphenicol	1.8	2.6
chlorbromuron	4.8	4.5
chlordane	6.4	7.5
chlordene	7.1	5.7
chlorflurecol	4.4	4.0
chlorimuron	1.6	3.2
chloroacetamide	0.9	0.6
chlorobenzene	4.1	4.0
chlorobenzene	4.1	4.0
chlorocyclohexane	4.1	4.3
chlorodibromomethane	3.6	3.8
chlorodifluoromethane	3.2	3.3
chloroethane	2.8	3.0
chloroethane	2.7	3.0
chloroethylene	3.1	3.2
chloroform	2.9	2.8
chloroneb	5.0	4.9
chloropham	4.9	4.1
chloropropylate	5.6	6.4
chlorothalonil	5.6	5.5
chlorothiazide	2.0	0.7
chlorotoluron	3.8	3.5
chloroxuron	5.0	5.2
chlorpropamide	3.3	3.6
chlorquinox	5.9	5.8
chlorsulfuron	0.7	2.3

cholanthrene	8.3	8.2
cholesterol	6.8	9.5
chrysene	7.5	7.7
chrysene	7.5	7.7
cinnamic acid	3.1	2.4
cis 1,2-dichloroethylene	2.9	3.5
cis-1,2-dimethylcyclohexane	6.1	5.1
cis-1,4-dimethylcyclohexane	6.2	5.1
cis-2-butene	3.8	3.2
cis-2-Heptene	5.6	4.8
cis-2-hexene	5.0	4.2
cis-2-pentene	4.3	3.7
cis-3-chloro-2-butenoic acid	2.1	1.8
cis-crotonic acid	1.4	1.1
citral	3.8	4.4
codeine	2.1	2.3
coronene	9.1	8.6
corticosterone	3.4	2.9
cortisone	2.3	1.6
cortisone acetate	3.3	2.5
cortisone-acetate	3.1	2.5
coumaphos	6.1	6.1
coumarin	3.2	2.7
cyanazine	3.0	3.0
cycloate	5.1	5.3
cycloheptane	5.3	4.5
cycloheptanol	2.6	3.2
cycloheptatriene	3.9	4.6
cycloheptene	4.9	4.5
cyclohexane	4.9	3.8
cyclohexanol	2.1	2.6
cyclohexanol acetate	3.4	3.4
cyclohexanone	2.3	2.5
cyclohexene	4.3	3.9
cyclooctane	5.9	5.1
cyclooctanol	3.0	2.5
cyclopentane	4.4	3.2
cyclopentene	3.8	3.2
cyclopropane	3.8	1.9
cyprazine	3.6	3.1
dacthal	6.0	6.0
daimuron	4.7	4.6
danazol	5.5	6.4
decachlorobiphenyl	9.2	11.7
decachlorodiphenyl ether	13.0	11.8
decalin	6.1	4.8
decanoic acid	5.1	4.8
delmadinone acetate	5.1	5.9
delta-hexachlorocyclohexane	5.2	6.4
deoxycorticosterone	4.1	4.1

deoxycorticosterone acetate	4.8	5.1
desmedipham	4.8	4.0
desmetryn	3.5	3.5
dexamethasone	2.2	2.8
dexamethasone-17-acetate	3.8	3.7
d-fenchone	3.6	3.7
di(2-ethylhexyl)-phthalate	8.7	10.2
diallate	6.0	6.4
diallyl phthalate	4.9	5.3
diazepam	4.6	5.2
diazinon	5.6	6.0
dibenz(a,h)anthracene	8.6	9.1
dibenzodioxin	6.0	6.4
dibenzofuran	5.9	5.8
dibenzofurane	5.9	4.9
dibenzo-p-dioxin	6.4	6.1
dibenzothiophene	6.1	5.6
dibromochloromethane	3.6	3.2
dibromomethane	2.9	3.2
dibutyl ether	4.4	4.5
dibutyl phthalate	6.1	6.7
dibutylphthalate	6.1	6.7
dichlormid	3.4	2.9
dichlorodifluoromethane	3.7	4.2
dichlorodiphenyldichloroethane	7.3	7.3
dichlorodiphenyldichloroethylene	8.0	7.5
dichlorodiphenyltrichloroethane	7.9	7.5
dichloromethane	2.6	3.0
diclofopmethyl	5.3	6.7
dieldrin	6.7	4.7
diethyl disulfide	4.4	4.2
diethyl ether	1.8	2.4
diethyl malonate	2.6	2.4
diethyl o-phthalate	4.1	4.6
diethyl phthalate	4.1	4.6
diethyl succinate	2.7	2.6
diethyl sulfide	3.2	3.9
diethylstilbestrol	4.3	6.0
difenoxuron	4.2	4.7
diflubenzuron	5.6	5.2
difluron	5.2	5.2
digitoxin	3.8	3.5
digoxin	2.5	2.7
diiodomethane	4.2	4.1
diisobutylphthalate	6.4	6.0
diisopropyl ether	2.8	2.8
diisopropyl ketone	3.0	3.3
diisopropyl sulfide	4.0	4.4
diisopropylketone	3.0	3.3
dimepiperate	5.6	5.3

dimetan	2.3	2.8
dimethametryn	4.8	4.8
dimethoate	2.1	2.2
dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	1.1	1.1
dimethyl carbate	2.8	2.7
dimethyl disulfide	3.2	3.1
dimethyl fumarate	0.7	1.5
dimethyl maleate	2.0	1.5
dimethyl oxalate	1.7	1.3
dimethyl phthalate	3.4	3.5
dimethyl sulfide	2.2	2.9
dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	5.9	6.0
dimethylsulfide	2.2	2.9
dimethylterephthalate	4.4	3.5
di-n-butyl succinate	4.7	4.7
dinoseb	4.7	5.2
diosgenin	7.6	7.6
dioxacarb	2.2	2.9
diphenamid	3.4	4.0
diphenyl ether	5.7	5.5
diphenyl phthalate	7.7	6.5
diphenylacetic acid	3.4	3.9
diphenylamine	5.0	4.6
diphenylcarbinol	3.8	3.8
diphenylmethane	5.8	5.9
dipropalin	3.9	6.7
dipropetryn	4.7	4.8
dipropyl ether	3.4	3.4
dipropyl sulfide	4.3	5.0
disulfoton	4.3	6.6
ditolyl ether	6.6	6.5
diuron	4.0	3.7
dl-1,2-diphenylethanol	3.8	4.6
d-limonene	5.7	6.0
dodecane	9.4	7.9
dodecanedioic acid	3.2	3.8
dodecanol	6.4	6.5
d-querticol	0.1	-2.4
dulcin	2.0	1.7
E-3-chloro-2-butenoic acid	2.1	1.5
endothall	0.9	0.0
epiandrosterone	4.7	5.2
epichlorohydrin	1.9	2.0
epitiostanol	6.3	6.5
equilenin	4.9	5.0
estradiol	5.2	4.6
estragole	4.7	5.2
estrone	2.0	4.5
ethalfluralin	7.4	7.2
ethane	4.4	2.7

ethanethiol	2.3	2.8
ethinyl-estradiol	5.0	5.4
ethiofencarb	3.7	4.4
ethiofencarb	3.7	4.4
ethion	7.3	7.5
ethirimol	2.8	3.6
ethisterone	5.3	6.0
ethofumesate	4.6	5.2
ethoxybenzene	4.1	4.0
ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	5.0	4.0
ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	6.0	6.2
ethyl 4-aminobenzoate	3.1	3.2
ethyl acetate	1.8	2.1
ethyl acrylate	2.5	2.7
ethyl acrylate	2.6	2.7
ethyl bromide	2.8	3.1
ethyl butyrate	3.1	3.2
ethyl caprinate	5.8	6.3
ethyl cinnamate	4.7	2.5
ethyl cyanoacetate	2.5	1.8
ethyl heptanoate	4.5	4.7
ethyl hexanoate	4.1	4.2
ethyl iodide	3.3	3.5
ethyl mercaptan	2.3	2.8
ethyl N-benzoyl-n-(3,4-dichlorophenyl)-dl-alaninate	5.4	6.1
ethyl nitrate	1.9	2.3
ethyl pelargonate	5.5	5.8
ethyl pentanoate	3.5	3.7
ethyl propionate	2.5	2.6
ethyl propyl ether	2.4	2.9
ethyl valerate	3.5	3.7
ethyl vinyl ether	2.6	3.2
ethylacetate	1.8	2.1
ethylbenzene	4.5	4.4
ethylbenzoate	4.1	4.0
ethyl-biscoumacetate	3.4	3.7
ethylbutyrate	3.0	3.5
ethyl-caproate	4.1	4.2
ethyl-caprylate	5.1	5.3
ethylcyclohexane	6.0	5.0
ethylene	4.1	2.9
ethyl-isopropyl-ether	2.3	2.6
ethynyl estradiol	4.8	5.4
etofenprox	10.1	8.7
eucalyptol	4.1	4.7
eugenol	3.3	3.8
fenbufen	4.8	3.7
fenfuram	4.1	3.3
fenobucarb	4.3	4.6
fenothiocarb	5.4	5.4

fenoxycarb	5.9	5.7
fensulfothion	4.0	4.1
fenthion	6.3	5.9
fenuron	2.1	2.4
flazasulfuron	1.8	2.6
flufenoxuron	7.7	8.8
flumethiazide	0.1	1.4
fluometuron	3.5	3.8
fluorene	5.9	5.4
fluorobenzene	3.5	3.6
fluorodifen	6.1	6.4
fluoromethalone	3.5	4.2
fluorotrichloromethane	3.8	4.4
flurbiprofen	5.3	5.1
fluridone	4.8	8.6
flurobenzene	3.5	3.6
Forchlorfenuron	3.8	3.1
furan	2.6	2.9
furan	2.6	2.9
furfural	1.8	2.8
furosemide	3.1	3.1
gentisin(sp)	2.6	3.3
glyburide	3.6	5.4
glyceryl triacetate	2.3	1.3
griseofulvin	4.0	3.8
guaiacol	2.4	2.1
haloperidol	5.1	6.7
halosulfuron	3.6	2.1
halothane	3.5	4.2
heptabarbital	2.6	3.2
heptachlor	7.4	7.1
heptachlor-epoxide	6.6	5.3
heptanal	3.7	3.6
heptane	6.2	5.3
heptanoic acid	3.4	3.2
heptylbenzene	7.3	7.0
hexachloro-1,3-butadiene	6.7	6.2
hexachlorobenzene	7.7	7.2
hexachlorocyclopentadiene	6.9	6.9
hexachloroethane	3.9	5.2
hexachloroethane(sp)	3.8	3.7
hexadecane	10.1	10.0
hexaflumuron	6.0	6.8
hexafluoroethane	6.0	4.5
hexamethylbenzene	6.3	6.2
hexanal	3.0	3.1
hexyl acetate	4.2	4.2
hexyl ethanoate	4.2	4.2
hexyl-4-aminobenzoate	5.1	5.3
hexylbenzene	7.0	6.5

hydrobenzoin	2.6	3.0
hydrochlorothiazide	2.2	1.4
hydrocinnamic acid	2.9	2.8
hydrocortisone	2.4	1.6
hydrocortisone tebutate	4.1	4.3
hydrocortisone-21-acetate	3.6	2.5
hydroflumethiazide	2.6	2.1
hydroxyisoandrosterone	3.9	3.9
hydroxyprogesterone-17alpha	4.8	4.3
ibuprofen	4.9	4.7
imazosulfuron	4.1	2.7
indane	4.8	4.2
indazole	2.8	2.8
indole	3.0	3.6
indoline	2.8	2.7
iodobenzene	4.5	4.6
iodoethane	3.3	3.5
iodofenphos	6.5	7.2
iodomethane	2.8	3.0
iorazepam	4.1	3.5
ipazine	4.6	4.8
isoamyl formate	3.3	3.2
isobutane	4.8	3.4
isobutene	4.1	3.4
isobutyl acetate	3.0	2.9
isobutyl formate	2.7	2.7
isobutylacetate	3.0	3.4
isobutylbenzene	5.9	5.1
isobutylformate	2.8	2.8
isobutyltoluene	5.9	5.7
isoflurane	3.1	3.0
isonicotinic acid	0.3	1.4
isopentanol	2.3	2.5
isopentyl acetate	3.6	3.4
isopentyl formate	3.3	3.2
isopentyl propionate	4.0	4.2
isophorone	2.8	4.4
isoprene	3.8	3.9
isoprocarb	3.6	4.0
isopropyl 4,4'-dibromobenzilate	7.8	7.0
isopropyl acetate	2.3	2.3
isopropyl ether	2.8	2.8
isopropyl formate	2.4	2.2
isopropyl methyl ketone	1.9	2.4
isopropyl nitrate	3.2	3.2
isopropyl phenylcarbamate	4.2	3.4
isopropyl tert-butyl ether	4.1	3.2
isopropylacetate	2.3	2.3
isopropylbenzene	5.0	4.7
isoproturon	3.6	3.8

isoquinoline	3.2	4.0
isouron	3.1	2.6
ketoprofen	4.2	3.7
khellin	2.8	3.6
L-carvone	3.8	4.7
leptophos	7.0	7.7
lidocaine	2.9	3.2
linalool	3.7	4.2
lindane	5.4	6.4
linuron	4.4	4.3
l-menthone	4.2	4.6
lufenuron	6.3	7.9
m-acetotoluidide	3.4	2.6
malonic acid diethyl ester	2.6	2.4
m-aminophenol	1.3	1.2
m-benzenedicarboxylic acid	2.3	1.0
m-bromobenzoic acid	3.3	3.1
m-bromophenol	2.5	2.9
m-bromotoluene	5.3	4.8
m-chloroaniline	3.1	3.3
m-chlorobromobenzene	5.0	4.9
m-chloroiodobenzene	5.0	5.3
m-chloronitrobenzene	4.4	4.1
m-chlorotoluene	5.3	4.5
m-cyanoaniline	2.7	2.4
m-cymene	5.2	5.2
m-diethylbenzene	5.5	5.4
mebendazole	2.0	3.3
meconin	2.8	2.5
medrogestone	6.0	6.8
mefluidide	2.9	3.1
megestrol acetate	5.1	5.8
menadione	4.1	3.1
menthol	4.1	4.6
menthone	4.1	4.6
meprobamate	2.0	1.6
methabenzthiazuron	4.2	3.0
methanethiol	2.2	2.3
methapyrilene	4.4	4.0
methazole	3.7	4.7
methiocarb	4.5	4.4
methomyl	1.5	1.5
methoprene	4.0	6.5
methoxsalen	4.3	5.0
methoxybenzene	3.8	3.5
methoxychlor	7.5	7.2
methoxyflurane	2.5	2.5
methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	7.1	6.7
methyl 2,4-dichlorophenoxyacetate	4.5	4.2
methyl 3-m-tolylcarbamoyloxyphenylcarbamate	4.5	4.0

methyl 4-aminobenzoate	2.4	2.7
methyl 4-hydroxybenzoate	2.5	2.1
methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	6.9	7.0
methyl acrylate	2.0	2.2
methyl benzoate	3.6	3.5
methyl butyl ether	2.7	2.9
methyl butylketone	2.5	3.1
methyl butyrate	2.6	2.6
methyl chloride	2.7	2.5
methyl decanoate (methyl caprate)	6.4	5.8
methyl hexanoate	3.7	3.7
methyl isopropyl ether	1.8	2.0
methyl laurate	6.1	6.8
methyl methacrylate	2.6	2.9
methyl n-butyl ether	2.7	2.9
methyl nonanoate	5.6	5.3
methyl octanoate (methyl caprylate)	5.1	4.7
methyl pentanoate	3.1	3.2
methyl phenyl ether	3.8	3.5
methyl propionate	1.9	2.1
methyl propyl ether	2.1	2.4
methyl tert-butyl ether	2.0	2.5
methyl valerate	3.1	3.2
methyl-4-aminobenzoate	2.5	2.7
methyl-4-methoxybenzoate	3.9	3.6
methyl-capronate	3.7	3.7
methylcyclohexane	5.6	4.5
methylcyclopentane	5.0	3.8
methyldymron	4.5	4.8
methylphenylsulfide	4.1	4.1
methylprednisolone	3.2	2.3
methyl-t-butyl ether	2.0	2.5
metobromuron	3.7	3.9
metolachlor	4.5	3.8
metolcarb	3.0	3.2
metoxuron	3.0	3.2
m-fluorobenzoic acid	2.8	2.4
m-fluorobromobenzene	4.4	4.5
m-hydroxybenzaldehyde	2.2	1.9
m-hydroxybenzyl alcohol	1.6	1.0
m-hydroxytoluene	2.4	2.5
mininoxidil	1.7	1.2
m-nitrobenzaldehyde	3.4	3.4
m-nitrobenzoic acid	2.5	2.3
m-nitrobenzyl alcohol	4.1	2.5
m-nitrobromobenzene	2.8	4.4
m-nitrophenol	2.1	2.1
monolinuron	3.6	3.6
monuron	3.0	3.1
m-terphenyl	6.2	7.3

m-toluic acid	3.3	2.7
m-toluidine	2.6	3.1
m-xylene	4.6	4.3
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	7.4	7.0
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine	7.1	7.4
N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	6.2	6.0
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	4.8	4.1
N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea	3.0	3.2
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	5.7	5.2
N-(4-chlorophenyl)-2,2-dimethylpentanamide	5.1	5.0
N'-(4-chlorophenyl)-N-methoxy-N-methylurea	3.5	3.6
N-(cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl)benzenamine	8.2	6.9
N, N'-diethylthiourea	2.5	2.9
N,N'-(2-hydroxyethyl)-1,4-diaminoanthraquinone	5.1	4.5
N,N-(2-hydroxyethyl)-4-phenylazoaniline	4.3	4.3
N,N-(2-hydroxyethyl)-4-phenylazoaniline	4.3	4.3
N,N-diethyl-2-(1-naphthyloxy)propionamide	4.7	4.9
N,N-dimethyl-2,2-diphenylacetamide	3.5	4.0
N,N-dimethyl-4-phenylazoaniline	6.8	6.2
N,N-dimethylaniline	3.7	3.9
N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea	3.4	3.8
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea	3.4	3.8
N,N'-dinitroethanediamine	1.8	1.8
N,N'-di-n-propyladipamide	1.4	2.8
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	4.8	4.9
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-propanamide (sufentanil)	4.6	4.4
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea	2.1	2.3
n-amyl-carbamate	2.2	2.6
naphthacene	7.8	7.7
naphthalene	4.8	4.8
napropamide	4.5	4.9
n-butyl benzoate	5.2	5.0
n-butyl mercaptan	3.9	3.8
n-butylbenzene	5.8	5.4
N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea	5.5	5.3
N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline	7.5	7.6
n-decane	8.2	6.9
neburon	5.3	5.3
n-heptyl carbamate	3.7	3.4
n-hexane	5.7	4.8
n-hexyl carbamate	3.1	3.1
nicosulfuron	1.3	0.9
nicotinic acid	0.6	1.4
nifedipine	4.7	5.7
nitralin	5.6	6.1
nitrapyrin	5.1	3.1
nitrobenzene	3.5	3.5
nitroethane	1.9	2.3
N-methyl-2,4,6,N-tetranitroaniline	4.2	4.7

n-octane	7.0	5.8
n-octylbenzene	8.2	7.5
nonanal	4.9	4.6
nonane	7.8	6.3
nonanoic acid	4.5	4.3
norethindrone	4.8	4.6
norethindrone acetate	4.8	5.4
norethisterone-acetate	5.2	5.2
norflurazon	4.1	4.8
noscapine	3.0	2.5
novaluron	6.0	5.9
n-pentadecane	11.2	9.5
N-phenyl-N[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)	4.3	5.3
n-propylbenzene	5.1	4.9
N-Sulfanilylsulfanilamide	3.3	2.4
N-tert-butylurea	0.5	0.7
n-tridecane	9.3	8.4
n-undecane	9.3	7.4
O-(2-chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate	5.6	5.9
O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate	7.4	7.3
O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphonothioate	8.1	7.7
O,O-diethyl O-4-nitrophenyl phosphorothioate	6.2	6.3
O,O-diethyl O-quinoxalin-2-yl phosphothioate	5.8	6.0
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	7.0	7.3
O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	5.7	6.1
O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	7.1	7.0
O,O-dimethyl O-4-nitrophenyl phosphorothioate	5.5	5.3
O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate	2.4	2.0
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	6.3	6.2
o,p'-dichlorodiphenyldichloroethane	7.7	7.3
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl O,O-diethyl phosphorothioate	6.3	6.6
o-acetoxybenzoic acid	2.2	2.1
o-aminophenol	0.5	0.9
o-benzenedicarboxylic acid	1.5	1.9
o-bromobenzoic acid	2.7	3.3
o-bromobenzyl alcohol	3.4	3.6
o-chloroacetanilide	2.5	2.6
o-chloroaniline	2.9	3.1
o-chloroanisole	4.2	4.1
o-chlorobiphenyl	6.2	6.0
o-chloroiodobenzene	5.3	5.3
o-chlorotoluene	4.3	4.5
octachlorodibenzofuran	11.5	10.8
octachlorodibenzo-p-dioxin	12.5	11.7
octafluorocyclobutane	5.7	5.8
octafluoropropane	6.3	5.1
octanal	4.1	4.1
octanoic acid	4.0	3.8
o-cymene	5.5	5.2
o-diethylbenzene	5.0	5.4

O-ethyl O-(4-nitrophenyl)phenylphosphonothioate	6.6	6.2
o-ethyltoluene	4.9	4.9
o-fluorobenzoic acid	2.1	2.6
o-hydroxyacetanilide	3.3	1.1
o-hydroxybenzamide	2.6	1.4
o-hydroxybenzyl alcohol	1.5	1.6
o-hydroxybiphenyl	3.9	4.0
o-hydroxytoluene	2.3	2.5
O-isobutyl carbamate	1.6	1.8
o-methoxybenzamide	2.5	2.7
o-methoxybenzoic acid	2.5	2.6
o-methoxyphenol	2.5	1.9
o-nitroacetanilide	3.0	2.5
o-nitrobenzaldehyde	3.4	3.7
o-nitrobenzoic acid	1.7	2.8
o-nitrobenzyl alcohol	2.8	3.0
o-nitrophenol	3.3	2.4
o-nitrotoluene	4.1	4.0
o-octyl carbamate	4.3	4.2
o-phenylenediamine	1.3	2.4
orbencarb	5.8	5.8
oryzalin	3.4	5.1
osthole	5.4	6.2
o-terphenyl	6.7	7.3
o-toluic acid	3.1	2.7
o-toluidine	2.5	3.1
o-tolylurea	1.9	1.5
oxasulfuron	3.5	2.5
oxazepam	4.1	2.5
oxycarboxin	3.2	3.0
o-xylene	4.7	4.3
p-acetotoluidide	2.5	2.6
p-acetoxy-acetanilide	2.1	2.0
p-aminobenzene sulphonamide	1.7	1.5
p-aminophenol	1.4	1.2
p-benzoquinone	2.0	2.6
p-bromobenzoic acid	3.5	3.1
p-bromobenzyl alcohol	3.4	3.3
p-bromoiodobenzene	5.8	5.5
p-bromophenyl urea	1.3	1.9
p-bromotoluene	4.9	4.8
p-chloroacetanilide	3.0	2.8
p-chloroaniline	2.9	3.3
p-chloroiodobenzene	5.5	5.3
p-chloronitrobenzene	4.1	4.1
p-chlorotoluene	4.8	4.5
p-chlorotoluene	4.8	4.5
p-cyanobenzoic acid	2.3	2.0
p-cymene	5.5	5.2
p-dichlorobenzene	4.9	4.7

p-diethylbenzene	5.4	5.4
p-difluorobenzene	3.7	3.7
pebulate	5.0	5.6
pelletierine	2.2	2.1
penbutolol	2.6	2.6
pencycuron	6.1	6.0
pendimethalin	7.3	6.5
pentachlorobenzene	6.6	6.5
pentachlorobutadiene	6.0	5.4
Pentachloroethane	4.4	4.5
pentachloronitrobenzene	6.6	6.7
pentachlorophenol	5.0	4.8
pentaerythrityl tetrabromide	5.6	5.6
pentafluorochloroethane	5.2	4.6
pentamethylbenzene	5.5	5.8
pentanal	2.6	2.5
pentane	5.0	4.2
pentanoic acid	2.4	2.2
pentyl 4-aminobenzoate	4.7	4.8
pentyl acetate	3.6	3.7
pentyl propanoate	4.0	4.2
pentylbenzene	6.4	6.0
pentylcyclopentane	7.8	5.6
perchloropropylene	5.9	5.4
permethrin	7.9	9.0
perthane	8.3	8.0
perylene	8.0	8.0
p-ethoxyacetanilide	2.6	2.8
p-ethyl hydroxybenzoate	3.0	2.6
p-ethylphenol	2.9	3.0
p-ethyltoluene	4.9	4.9
p-fluorobenzoic acid	2.6	2.4
p-fluorobenzyl chloride	4.3	4.3
phenacetin	2.7	2.8
phenallymal	2.5	2.4
phenanthrene	6.3	6.3
phenanthridine	3.7	5.5
phenetole	4.1	4.0
phenmedipham	4.7	4.0
phenobarbital	2.4	2.0
phenobenzuron	4.9	6.6
phenol	1.7	2.0
phenolphthalein	3.0	3.7
phenothrin	7.0	8.7
phenyl glycidyl ether	3.5	3.0
phenylacetic acid	2.3	2.6
phenylmethanol	2.1	2.4
phenytoin	3.2	4.7
phorate	5.8	6.1
phthalazine	1.7	3.7

phthalonitrile	3.2	3.0
p-hydroxyacetanilide	1.3	0.8
p-hydroxyacetophenone	2.1	1.3
p-hydroxybenzaldehyde	2.2	1.9
p-hydroxybenzyl alcohol	2.1	1.0
p-hydroxytoluene	2.4	2.5
picene	6.3	9.1
picric acid	2.3	2.9
pimilic acid	1.2	1.2
pindone	5.0	2.8
piperine	3.9	3.4
piperonal	3.3	1.5
pirimicarb	2.9	2.1
p-isopropylbenzoic acid	3.9	3.5
p-methoxyacetanilide	1.5	2.3
p-methoxybenzaldehyde	3.2	3.4
p-methoxyphenol	1.9	2.1
p-methylacetophenone	4.3	3.2
p-methylbenzyl alcohol	2.6	2.9
p-nitroacetanilide	1.7	2.3
p-nitrobenzaldehyde	2.9	3.4
p-nitrobenzoic acid	2.0	2.3
p-nitrobenzyl alcohol	3.0	2.5
p-nitrophenol	2.1	2.1
p-N-methylhydroxyaniline	2.2	2.1
p-phenylazoaniline	4.6	4.9
p-phenylenediamine	1.2	1.9
p-propylphenol	3.8	3.5
prasterone	4.3	4.6
prasterone acetate	4.9	5.4
prednisolone	2.1	1.7
prednisolone acetate	3.6	2.6
prednisone	3.1	1.6
prednisonone-21-trimethylacetate	3.6	3.7
pregnenolone	4.9	5.7
primidone	1.8	2.6
prodiamine	7.7	6.8
profluralin	8.2	6.9
progesterone	5.1	5.6
promecarb	4.3	4.5
prometon	3.4	3.3
prometryn	4.5	4.2
propachlor	3.6	3.2
propane	4.6	3.2
propanil	4.2	3.9
propazine	3.7	3.9
propene	4.1	3.0
propionanilide	2.7	2.7
propiophenone	3.6	3.3
propoxur	2.9	3.5

propyl 4-aminobenzoate	3.6	3.7
propyl 4-hydroxybenzoate	3.4	3.1
propyl acetate	2.5	2.7
propyl benzoate	4.4	4.5
propyl butyrate	3.7	4.0
propyl formate	2.3	2.5
propyl isopropyl ether	3.1	3.8
propyl propanoate	3.1	3.2
propyl propionate	3.1	3.2
propylcyclopentane	6.5	4.9
propyne	2.2	2.5
propyne	2.8	2.5
prostaglandin E2	3.3	4.4
p-terphenyl	6.3	7.3
p-toluic acid	3.0	2.7
p-toluidine	2.8	3.1
p-xylene	4.6	4.3
pyracarbolid	3.4	3.5
pyrazon	3.0	2.3
pyrazosulfuron-ethyl	3.3	2.0
pyrene	7.0	6.6
pyrrole	1.9	2.2
pyrrole	1.9	2.2
quinoline	3.1	4.0
quinone	1.7	1.3
quintozene	6.5	6.7
rimsulfuron	3.8	1.7
ronnel	5.5	6.5
rotenone	4.6	5.9
S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate	5.9	6.1
S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethyl phoshorodithioate	5.3	5.1
S-2,3,3-trichloroallyl diisopropylthiocarbamate	6.5	6.2
salbutamol	1.1	-1.5
salicin	0.4	-1.1
salicyl alcohol	1.5	1.0
salicylaldehyde	2.6	1.9
santonin	3.6	3.3
sebacic acid	2.2	2.7
secbumeton	3.3	3.6
sec-butylbenzene	5.5	5.3
siduron	4.2	4.2
simazine	3.6	3.5
simetryn	3.6	3.8
styrene	4.3	4.4
styrene oxide	3.3	3.2
suberic acid	1.5	1.7
succinic acid	-0.1	-0.4
sulfabenzamide	2.9	3.0
sulfacetamide	1.3	1.2

sulfacytine	2.3	2.0
sulfadiazine	2.8	1.9
sulfadimethoxine	2.3	2.2
sulfaethidole	1.7	2.7
sulfamerazine	2.6	2.4
sulfameter	2.0	2.0
sulfamethazine	2.4	2.9
sulfamethizole	2.2	2.2
sulfamethomidine	2.8	2.5
sulfamethoxazole	2.8	2.5
sulfamethoxypyridazine	3.1	2.5
sulfamethylthiazole	1.6	2.5
sulfamoxole	2.1	3.2
sulfaperine	2.0	2.4
sulfapyrazine	3.0	1.9
sulfapyridine	2.9	2.7
sulfaquinoxaline	4.0	3.4
sulfathiazole	2.7	2.0
sulfathiozole	2.3	2.0
sulfisomidine	1.6	2.9
sulfisoxazole	2.9	3.0
sulfometuron-methyl	2.3	2.8
sulfosulfuron	3.1	2.5
t-amylbenzene	5.9	5.5
tebuthiuron	2.1	2.3
teflubenzuron	6.5	6.2
terbumeton	3.7	3.5
terbuthylazine	4.3	4.1
terbutryn	4.7	4.5
terbutryne	4.6	5.8
tert-amyl carbamate	1.8	2.2
tert-butyl bromide	4.1	3.7
tert-butyl chloride	3.2	3.6
tert-butylbenzene	5.4	5.0
testosterone	4.3	4.6
testosterone acetate	5.8	5.4
testosterone propionate	6.0	5.9
tetrabromomethane	4.5	5.0
tetrachloroethene	4.6	4.8
tetrachloroethylene	4.5	4.8
tetrachloroguaiacol	4.8	4.6
tetrachloromethane	4.1	4.5
tetradecane	9.7	9.0
tetrafluoroethylene	4.5	3.0
tetrafluoromethane	5.4	4.0
tetrahydropyran	1.8	2.9
tetramethysuccinic acid	1.9	0.9
theophylline	0.9	-0.4
thiazafluron	2.5	2.0
thioanisole	4.1	4.1

thiobencarb	5.7	5.8
thiofanox	2.9	3.2
thiophene	3.2	2.7
thymine	3.0	0.2
thymol	3.7	3.8
tolbutamide	3.5	3.9
toluene	4.0	3.9
tranid	2.2	1.9
trans-1,2-dimethylcyclohexane	6.1	5.1
trans-1,4-dimethylcyclohexane	6.2	5.1
trans-2-butene	3.8	3.2
trans-2-heptene	5.6	4.5
trans-2-pentene	4.3	3.7
trans-azobenzene	5.7	5.7
triadimefon	4.6	4.2
triamcinolone	2.1	0.9
triamcinolone diacetate	3.1	2.6
triasulfuron	3.1	2.6
triazolam	4.1	5.7
tribromomethane	3.7	3.9
trichlorfon	1.2	1.0
trichlormethiazide	2.1	2.5
trichloroacetaldehyde	2.4	2.2
trichloroacetic acid	2.2	1.9
trichloroehylene	3.7	4.2
trichloroethylene	3.8	4.2
trichlorofluoromethane	3.8	3.6
trichloromethane	2.9	3.5
trichloronitromethane	3.7	3.0
tricyclazole	2.4	3.6
tridecanoic acid	5.1	6.4
trietazine	4.8	4.6
triflumuron	6.5	5.9
trifluoromethane	3.0	3.1
trifluoromethylbenzene	4.3	3.2
trifluralin	7.7	7.6
trimethoprim	2.1	2.1
trinitroglycerine	4.0	3.9
triphenylene	6.9	7.7
undecanedioic acid	1.8	3.3
undecanoic acid	5.2	5.3
valeraldehyde	2.6	2.5
veratrole	3.1	3.6
vernolate	5.0	5.6
vinyl acetate	2.4	2.3
vinyl chloride	2.6	3.2
warfarin	4.0	4.2
XMC	3.5	3.6
xylylcarb	3.6	3.6
Z-3-chloro-2-butenoic acid	1.7	1.8

APPENDIX C. Experimental, SCRACTH-predicted and GSE-predicted aqueous solubility values for 883 compounds along with their partition coefficient values (ClogP) obtained from EPI suite.

		logS_w(M)		
Name	**ClogP**	**Exp**	**SCRATCH**	**GSE**
(+)a-(3-benzoylphenyl)propionic acid	3.0	-3.7	-3.1	-3.2
(2,4,5-trichlorophenoxy)acetic acid	3.3	-3.0	-3.4	-4.1
(2,4-dichlorophenoxy)acetic acid	2.6	-2.5	-2.8	-3.3
(4-chloro-2-methylphenoxy)acetic acid	2.5	-2.5	-2.4	-3.0
(4-chloro-o-tolyloxy)acetic acid	2.5	-2.5	-2.4	-3.0
(d) 1,2-diphenyl-1,2-dihydroxyethane	2.1	-1.9	-2.4	-2.8
(d) 2-(m-chlorophenoxy)propanoic acid	2.4	-2.2	-2.2	-2.6
(d) methylenebisthiopropionic acid	0.6	-1.8	-0.8	-0.6
(dl) 1,2-diphenyl-1,2-dihydroxyethane	2.1	-1.9	-2.4	-2.5
(dl) 2-(m-chlorophenoxy)propanoic acid	2.4	-2.2	-2.2	-2.8
(dl) menthol	3.4	-2.5	-2.8	-2.9
(dl) methylenebisthiopropionic acid	0.6	-1.8	-0.8	-1.4
(l) menthol	3.4	-2.5	-2.8	-3.1
1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	2.9	-3.6	-3.6	-3.0
1-(methylamino)-9,10-anthracenedione	4.1	-6.3	-6.0	-5.0
1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)	6.8	-7.8	-7.3	-7.1
1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene	5.7	-6.5	-6.5	-5.8
1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene)	6.7	-6.5	-6.4	-6.5
1,1'-(2,2-dichloroethylidenebis(4-chlorobenzene)	5.9	-6.6	-6.2	-6.2
1,1,1-trichloroethane	2.7	-2.0	-2.2	-2.2
1,1,1-trifluoro-n-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide	4.2	-3.8	-3.8	-4.9
1,1,2,2-tetrachlorodifluoroethane	3.4	-3.2	-3.2	-2.9
1,1,2,2-tetrachloroethane	2.2	-1.8	-1.9	-1.7
1,1,2-trichloroethane	2.0	-2.1	-1.7	-1.5
1,1,2-trifluoro-1,2,2-trichloroethane	3.1	-3.0	-3.1	-2.6
1,10-decanediol	2.7	-2.1	-3.2	-2.7
1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene	6.0	-6.9	-6.5	-6.1
1,1-dichloroethane	1.8	-1.3	-1.4	-1.3
1,1-difluoro-1-chloroethane	2.1	-1.9	-1.9	-1.6
1,1-dimethyl-3-phenylurea	1.4	-1.6	-1.7	-1.9
1,2,3,4-tetrachlorobenzene	4.6	-4.6	-4.3	-4.3
1,2,3,4-tetrahydronaphthlene	4.0	-3.4	-3.4	-3.5
1,2,3,5-tetrachlorobenzene	4.6	-4.6	-4.3	-4.3
1,2,3,5-tetrafluorobenzene	2.8	-2.3	-2.3	-2.3
1,2,3,6,7,8-hexahydropyrene	6.1	-6.0	-6.7	-6.7
1,2,3-trichlorobenzene	3.9	-4.0	-3.5	-3.7
1,2,3-trimethylbenzene	3.6	-3.2	-3.1	-3.1
1,2,4,5-tetrabromobenzene	5.6	-7.0	-6.3	-6.6
1,2,4,5-tetrachloro-3-nitrobenzene	4.4	-5.1	-4.7	-4.6
1,2,4,5-tetrachlorobenzene	4.6	-5.6	-4.6	-5.3
1,2,4,5-tetrafluorobenzene	2.8	-2.4	-2.3	-2.3
1,2,4,5-tetramethylbenzene	4.2	-4.6	-3.8	-4.2

1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene	5.2	-6.7	-7.2	-5.9
1,2,4-trimethylbenzene	3.6	-3.3	-3.1	-3.1
1,2:3,4-dibenzanthracene	6.7	-8.2	-9.2	-8.8
1,2:5,6-dibenzanthracene	6.7	-8.4	-9.2	-8.7
1,2-benzacenaphthene (fluoranthene)	4.9	-5.9	-5.2	-5.3
1,2-benzanthracene	5.5	-7.4	-6.9	-6.4
1,2-benzofluorene	5.2	-6.7	-5.8	-6.3
1,2-benzopyrene	6.1	-7.6	-7.5	-7.2
1,2-bromochlorobenzene	3.5	-3.6	-3.2	-3.0
1,2-chloronitrobenzene	2.5	-2.6	-2.4	-2.1
1,2-dibromobenzene	3.8	-3.5	-3.5	-3.3
1,2-dibromoethane	2.0	-1.7	-1.8	-1.5
1,2-dibromotetrafluoroethane	3.0	-4.9	-3.2	-2.5
1,2-dicarbomethoxybenzene	1.7	-1.7	-1.8	-1.2
1,2-dichlorobenzene	3.3	-3.3	-2.9	-2.8
1,2-dichloroethane	1.8	-1.3	-1.6	-1.3
1,2-dichloropropane	2.3	-1.6	-1.8	-1.7
1,2-dichlorotetrafluoroethane	2.8	-2.7	-3.0	-2.3
1,2-difluorobenzene	2.4	-1.0	-2.0	-1.9
1,2-diiodobenzene	4.3	-4.2	-4.2	-3.8
1,2-dinitrobenzene	1.6	-2.5	-2.5	-2.1
1,2-diphenylethane	4.7	-4.6	-4.4	-4.5
1,3,5-trichlorobenzene	3.9	-3.8	-3.9	-3.8
1,3,5-trimethylbenzene	3.6	-3.4	-3.3	-3.1
1,3,5-trinitro-1,3,5-triazacyclohexane	0.7	-3.6	-2.4	-2.0
1,3,5-trinitrobenzene	1.5	-2.9	-2.9	-1.8
1,3-bromochlorobenzene	3.5	-3.2	-3.2	-3.0
1,3-butadiene	2.0	-1.9	-1.4	-1.5
1,3-dibromobenzene	3.8	-3.5	-3.5	-3.3
1,3-dibromopropane	2.5	-2.1	-2.3	-2.0
1,3-dicarbomethoxybenzene	1.7	-2.8	-1.8	-1.6
1,3-dichlorobenzene	3.3	-3.1	-2.9	-2.8
1,3-difluorobenzene	2.4	-2.0	-2.0	-1.9
1,3-diiodobenzene	4.3	-4.6	-4.2	-3.9
1,3-dinitrobenzene	1.6	-2.5	-2.2	-1.8
1,3-diphenylurea	3.0	-3.2	-3.7	-4.6
1,3-nitrochlorobenzene	2.5	-2.8	-2.4	-2.2
1,4-bromochlorobenzene	3.5	-3.6	-3.2	-3.4
1,4-bromoiodobenzene	4.1	-4.6	-4.0	-4.2
1,4-cyclohexadiene	2.8	-2.1	-2.1	-2.2
1,4-diamino-2-methoxyanthraquinone	3.2	-5.7	-5.4	-4.9
1,4-diaminoanthraquinone	3.2	-5.9	-5.3	-4.5
1,4-dibromobenzene	3.8	-4.0	-3.8	-3.9
1,4-dicarbomethoxybenzene	1.7	-4.0	-1.8	-2.3
1,4-dichloro-2,5-dimethoxybenzene	3.4	-4.4	-3.3	-4.0
1,4-dichlorobenzene	3.3	-3.3	-2.9	-3.1
1,4-dihydroxybenzene	1.0	-0.2	0.2	-2.1
1,4-diiodobenzene	4.3	-5.4	-4.9	-4.9
1,4-dimethylnaphthalene	4.3	-4.1	-4.3	-3.8
1,4-dinitrobenzene	1.6	-3.4	-2.8	-2.6

1,4-nitrochlorobenzene	2.5	-2.8	-2.6	-2.5
1,4-pentadiene	2.5	-2.1	-2.5	-2.0
1,5-dichloro-3-oxapentane	1.6	-0.9	-1.3	-1.1
1,8-dimethylnaphthalene	4.3	-4.8	-4.3	-4.1
10H-phenothiazine	3.8	-5.1	-5.5	-4.9
17-methyltestosterone	3.7	-4.0	-4.3	-4.6
1a,2a,3ß,4a,5a,6ß-hexachlorocyclohexane	4.3	-4.6	-4.9	-4.6
1-aminoanthraquinone	3.5	-5.9	-5.1	-5.3
1-bromo-2-chloroethane	1.9	-1.3	-1.7	-1.4
1-bromobutane	2.7	-2.2	-2.4	-2.1
1-bromoheptane	4.1	-4.4	-4.0	-3.6
1-bromohexane	3.6	-3.8	-3.5	-3.1
1-bromonaphthalene	4.1	-4.3	-4.0	-3.6
1-bromooctane	4.6	-5.1	-4.5	-4.1
1-bromopentane	3.1	-3.1	-2.9	-2.6
1-butene	2.2	-2.4	-1.8	-1.7
1-butyne	1.5	-1.3	-1.3	-1.0
1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene	6.8	-6.6	-7.3	-6.8
1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene	6.0	-6.4	-6.2	-6.0
1-chlorodibenzodioxin	5.0	-5.7	-5.8	-5.3
1-chloronaphthalene	3.8	-4.0	-3.7	-3.3
1-decanol	3.8	-3.6	-3.9	-3.3
1-decene	5.1	-5.4	-5.0	-4.6
1-heptanethiol	3.7	-4.2	-3.7	-3.2
1-heptanol	2.3	-1.8	-2.1	-1.8
1-heptene	3.6	-3.7	-3.4	-3.1
1-hexanol	1.8	-1.2	-1.6	-1.3
1-hexene	3.2	-3.2	-2.9	-2.6
1-iodonaphthalene	4.3	-4.5	-4.5	-3.8
1-methylnaphthalene	3.7	-3.8	-3.6	-3.2
1-naphthaleneacetamide	1.7	-3.7	-3.5	-2.8
1-naphthaleneacetic acid	2.6	-2.6	-3.3	-3.2
1-naphthoic acid	3.1	-3.3	-3.3	-3.9
1-naphthyl methylcarbamate	2.4	-3.3	-3.4	-3.0
1-naphthylamine	2.3	-1.9	-2.6	-2.0
1-nitronaphthalene	3.0	-4.3	-3.5	-2.8
1-nonene	4.6	-5.1	-4.4	-4.1
1-octene	4.1	-4.4	-3.9	-3.6
1-pentadecanol	6.2	-6.3	-6.8	-5.9
1-propanethiol	1.8	-1.6	-1.6	-1.3
1-tetradecanol	5.8	-6.1	-6.1	-5.4
2-(1,3-dioxolan-2-yl)phenyl methylcarbamate	0.3	-1.6	-3.2	-0.6
2-(1'-cyclohexenyl)cyclohexanone	3.7	-2.8	-3.4	-3.2
2-(1-methylethyl)phenyl methylcarbamate	2.4	-2.7	-2.6	-2.6
2-(2,4,5-trichlorophenoxy)propanoic acid	3.7	-3.1	-3.8	-4.7
2-(2,4-dichlorophenoxy)propanoic acid	3.0	-2.8	-3.0	-3.4
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	3.2	-5.2	-3.9	-3.7
2-(4-chloro-2-methylphenoxy)propanoic acid	2.9	-2.4	-2.8	-3.1

2-(6-methoxy-2-naphthyl)propionic acid	3.1	-4.2	-3.4	-4.0
2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	9.6	-10.4	-11.2	-10.6
2,2',3,3',5,5',6,6'-octachlorobiphenyl	8.9	-9.5	-10.7	-9.8
2,2',3,3',5,5',6-heptachlorobiphenyl	8.3	-8.6	-9.3	-8.7
2,2',3,3',6,6'-hexachlorobiphenyl	7.6	-7.9	-8.4	-8.0
2,2',4,5,5'-pentachlorobiphenyl	7.0	-7.3	-7.6	-7.0
2,2',4',5-tetrachlorobiphenyl	6.3	-7.3	-6.8	-6.2
2,2,4-trimethylpentane	4.1	-4.7	-3.3	-3.6
2,2-dimethyl-1-propanol	1.2	-0.4	-0.6	-0.7
2,2-dimethylbutane	3.2	-3.7	-2.6	-2.7
2,2-dimethylpentane	3.7	-4.4	-3.1	-3.2
2,2-dimethylpropane	2.7	-3.3	-2.1	-2.2
2,2-dimethylpropanoic acid (pivalic acid)	1.5	-0.7	-0.1	-1.1
2,3,4,5,6-pentachlorobiphenyl	7.0	-7.9	-7.9	-7.5
2,3,4,5-tetrachlorobiphenyl	6.3	-7.3	-6.8	-6.5
2,3,4-trimethylpentane	4.1	-4.7	-3.1	-3.5
2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione	2.2	-3.0	-4.4	-4.4
2,3,6-trichlorophenylacetic acid	3.4	-3.1	-3.7	-4.2
2,3-benzofluorene	5.2	-8.0	-5.9	-6.6
2,3-dichloro-1,4-naphthalenedione	2.7	-6.4	-5.1	-3.9
2,3-dichlorophenol	2.8	-1.7	-1.4	-2.6
2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	2.3	-2.8	-3.4	-3.1
2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	1.4	-2.3	-2.5	-1.9
2,3-dimethylbutane	3.1	-3.6	-2.4	-2.6
2,3-dimethylnaphthalene	4.3	-4.9	-4.3	-4.6
2,3-dimethylphenol	2.6	-1.4	-1.2	-2.6
2,3-dinitrotoluene	2.2	-2.8	-2.8	-2.0
2,4,5,6-tetrachloro-1,3-benzenedicarbonitile	3.7	-5.6	-5.3	-5.4
2,4,5-trichlorobiphenyl	5.7	-6.2	-6.0	-5.7
2,4,5-trichlorophenol	3.5	-2.2	-2.2	-3.4
2,4,6-N-tetranitroethylaniline	2.1	-3.7	-5.6	-2.3
2,4,6-tribromophenol	4.2	-3.7	-3.3	-4.4
2,4,6-trichlorobiphenyl	5.7	-6.0	-6.3	-5.6
2,4,6-trimethyl-1,3,5-trioxane	0.7	-0.1	-2.0	-0.2
2,4,6-trimethylpyridine	2.5	-0.5	-2.3	-1.9
2,4,6-trinitroresorcinol	1.1	-1.7	-1.5	-2.1
2,4,6-trinitrotoluene	2.0	-3.2	-3.8	-2.0
2,4,6-tri-tert-butylphenol	6.4	-3.9	-6.5	-7.0
2,4-dibromophenol	3.3	-2.1	-2.3	-2.9
2,4-dichlorophenol	2.8	-1.6	-1.4	-2.5
2,4-dichlorophenyl 4-nitrophenyl ether	4.3	-5.5	-5.9	-4.3
2,4-dimethylpentane	3.6	-4.3	-2.9	-3.1
2,4-dinitrochlorobenzene	2.3	-4.4	-3.0	-2.0
2,4-dinitrophenol	1.7	-1.8	-1.5	-2.1
2,4-dinitrotoluene	2.2	-2.8	-2.8	-2.1
2,5-dichlorophenol	2.8	-1.9	-1.4	-2.6
2,5-dimethylaniline	2.2	-1.3	-1.8	-1.7
2,5-dimethylphenol	2.6	-1.5	-2.1	-2.6
2,5-dinitrophenol	1.7	-2.7	-1.5	-2.1

2,6-dichloro-4-benzenamine	2.4	-2.3	-2.5	-3.6
2,6-dichloro-4-nitroaniline	2.8	-4.5	-2.8	-3.9
2,6-dichlorobenzonitrile	2.8	-3.9	-3.2	-3.5
2,6-dichlorobiphenyl	5.1	-5.0	-5.5	-4.6
2,6-dichlorophenol	2.8	-1.9	-1.5	-2.7
2,6-dimethylnaphthalene	4.3	-4.9	-4.3	-4.6
2,6-dimethylphenol	2.6	-1.3	-1.5	-2.3
2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	5.3	-6.3	-5.8	-5.0
2,6-di-tert-butyl-4-methylphenol	5.0	-5.6	-5.0	-5.0
2,6-di-tert-butylphenol	4.5	-4.9	-4.4	-4.1
2,7-dimethylnaphthalene	4.3	-4.9	-4.3	-4.5
2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	2.8	-5.5	-4.7	-3.9
2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	4.6	-4.2	-4.3	-5.9
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	2.5	-3.2	-3.8	-3.4
2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	-1.5	-1.1	0.3	0.4
2-aminobenzoic acid	1.4	-1.6	-1.1	-2.1
2-bromo-2-chloro-1,1,1-trifluoroethane	2.3	-1.7	-2.4	-1.8
2-bromonaphthalene	4.1	-4.4	-4.0	-3.9
2-bromopropane	2.1	-1.6	-1.6	-1.6
2-butanethiol	2.2	-1.8	-1.8	-1.7
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	5.2	-6.5	-6.6	-5.3
2-chloro-6-(trichloromethyl)pyridine	3.4	-3.5	-3.5	-3.2
2-chlorobenzoic acid	2.2	-1.9	-2.0	-2.8
2-chlorobiphenyl	4.4	-4.6	-4.4	-4.0
2-chlorodibenzodioxin	5.0	-5.8	-5.8	-5.1
2-chloro-n-(2,6-diethylphenyl)-n-(methoxymethyl)acetamide	3.4	-3.1	-1.9	-3.0
2-chloronaphthalene	3.8	-4.1	-3.7	-3.6
2-chloro-N-isopropyl N-phenylacetamide	2.4	-2.5	-1.5	-2.5
2-chlorophenol	2.2	-0.7	-0.7	-1.7
2-chloropropane	2.0	-1.4	-1.5	-1.5
2-cyclohexyl-4,6-dinitrophenol	4.5	-4.2	-4.6	-4.8
2-heptanone	1.7	-1.4	-1.9	-1.2
2-hexanone	1.2	-0.8	-1.4	-0.7
2-hydroxybenzoic acid	2.2	-1.8	-0.5	-3.1
2-iodobenzoic acid	2.7	-2.7	-3.0	-3.6
2-isopropoxyphenyl N-methylcarbamate	1.9	-2.1	-2.3	-2.0
2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide	2.9	-3.6	-2.7	-2.7
2-methyl-1,3-butadiene	2.6	-2.0	-2.1	-2.1
2-methyl-1-butene	2.7	-2.7	-2.1	-2.2
2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime	1.4	-1.5	-1.5	-1.6
2-methyl-2-butene	2.6	-2.6	-1.8	-2.1
2-methyl-4,6-dinitrophenol	2.3	-3.0	-1.2	-2.4
2-methylbutane	2.7	-3.2	-1.9	-2.2
2-methylfuran	1.9	-1.4	-1.6	-1.4
2-methylheptane	4.2	-4.5	-3.8	-3.7
2-methylhexane	3.7	-4.6	-3.2	-3.2

2-methylnaphthalene	3.7	-3.8	-3.6	-3.3
2-methylpentane	3.2	-3.8	-2.7	-2.7
2-naphthoic acid	3.1	-3.6	-3.3	-4.2
2-naphthylamine	2.3	-4.3	-2.6	-2.6
2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	3.8	-5.2	-5.4	-4.0
2-nitro-5-methylphenol	2.5	-2.8	-1.3	-2.0
2-nitroaniline	2.0	-2.0	-1.3	-2.0
2-octanone	2.2	-2.2	-2.4	-1.7
2-pentanol	1.3	-0.3	-0.8	-0.8
2-pentanone	0.8	-0.3	-0.8	-0.2
2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate	4.5	-5.5	-5.7	-4.4
3-(3,4-dichlorophenyl)-1,1-dimethylurea	2.7	-3.7	-3.3	-3.5
3-(4-chlorophenyl)-1,1-dimethylurea	2.0	-2.9	-2.5	-3.0
3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	0.3	-1.9	-2.0	-0.9
3(n-octyloxy)-1,2-propanediol	2.3	-1.9	-1.7	-1.8
3-(p-tolyl-4-sulfonyl)-1-butyl urea	2.4	-3.4	-3.5	-3.0
3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime	2.2	-1.6	-1.8	-2.0
3,3-dimethyl-2-butanone	1.1	-0.7	-0.9	-0.6
3,3-dimethylpentane	3.7	-4.2	-3.1	-3.2
3,3'-di-tert-butyl-5,5'-dimethyl-2,2-dihydroxydiphenylmethane	8.0	-7.2	-7.4	-8.5
3,4-benzophenanthrene	5.5	-8.1	-6.9	-5.4
3,4-benzopyrene	6.1	-8.2	-7.2	-7.2
3,4-dichloro-2-methoxybenzoic acid	2.1	-1.4	-3.0	-2.8
3,4-dichlorophenol	2.8	-1.2	-1.6	-2.7
3',4'-dichloropropionanilide	2.9	-3.2	-3.0	-3.0
3,4-dimethylisoxazol 5-sulphanylamide	1.0	-2.9	-2.9	-2.0
3,4-dimethylphenol	2.6	-1.4	-2.1	-2.5
3,4-dimethylphenyl methylcarbamate	2.3	-2.6	-2.5	-2.3
3,4-dinitrotoluene	2.2	-3.3	-2.8	-2.0
3,5,6-trichloro-2-pyridinyloxyacetic acid	2.5	-2.8	-2.8	-3.3
3,5-dibromo-4-hydroxybenzonitrile	3.4	-3.3	-2.9	-4.5
3,5-dichlorobenzoic acid	3.2	-3.1	-3.1	-4.3
3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	3.6	-4.2	-3.6	-4.4
3,5-dichlorophenol	2.8	-1.5	-1.9	-2.7
3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate	2.4	-3.3	-3.1	-2.6
3,5-dimethylphenol	2.6	-1.4	-1.5	-2.5
3,5-dinitrobenzoic acid	1.5	-2.2	-2.6	-2.8
3,6-dichloro-2-methoxybenzoic acid	2.1	-1.4	-3.0	-2.5
3-amino-2,5-dichlorobenzoic acid	1.9	-2.5	-2.5	-3.2
3-aminobenzoic acid	1.0	-1.4	-1.0	-2.0
3-chlorobenzoic acid	2.5	-2.5	-2.0	-3.3
3-chlorophenol	2.2	-0.7	-0.9	-1.7
3-heptanone	1.7	-1.4	-1.9	-1.2
3-hexanone	1.2	-0.8	-1.3	-0.7
3-hydroxybenzoic acid	1.4	-1.3	-0.5	-2.7
3-iodobenzoic acid	3.0	-3.3	-3.0	-4.2
3-methyl-1-butene	2.6	-2.7	-2.2	-2.1

3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	2.0	-2.1	-2.9	-1.7
3-methylheptane	4.2	-5.2	-3.8	-3.7
3-methylpentane	3.2	-3.7	-2.7	-2.7
3-methylthiophene	2.4	-2.4	-1.5	-1.9
3-nitroaniline	1.5	-2.1	-1.3	-1.9
3-nitrotoluene	2.4	-2.4	-2.3	-1.9
3-pentanol	1.3	-0.2	-0.8	-0.8
3-pentanone	0.8	-0.3	-0.8	-0.2
4-(1,1-dimethylethyl)-n-(1-methylpropyl)-2,6-dinitrobenzeneamine	5.2	-5.5	-5.4	-5.1
4-(2,4,5-trichlorophenoxy)butanoic acid	4.2	-3.8	-4.7	-4.6
4-(2,4-dichlorophenoxy)butyric acid	3.6	-3.7	-3.9	-4.0
4-(4-chloro-2-methylphenoxy)butanoic acid	3.5	-3.7	-3.7	-3.8
4-(4-nitrophenylazo)aniline	3.6	-5.9	-4.3	-5.0
4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide	2.7	-5.1	-4.9	-3.4
4,4'dihydroxydiphenyl-2,2-propane	3.6	-3.3	-3.5	-4.5
4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	3.6	-4.5	-3.2	-4.5
4-aminoacetophenone	0.8	-1.6	-0.6	-1.1
4-aminobenzoic acid	1.0	-1.4	-1.3	-2.1
4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide	0.2	-3.3	-2.7	-1.3
4-aminopyridine	-0.1	-0.1	-0.2	-0.7
4-bromophenol	2.4	-1.1	-1.5	-2.3
4-chloroazobenzene	4.8	-5.7	-5.2	-4.9
4-chlorobenzoic acid	2.5	-3.3	-2.3	-4.2
4-chlorobiphenyl	4.4	-5.1	-4.7	-4.4
4-chlorophenol	2.2	-0.7	-1.1	-1.8
4-chlorophenoxyacetic acid	2.0	-2.3	-1.8	-2.8
4-heptanone	1.7	-1.6	-1.9	-1.2
4-hexylresorcinol	4.0	-2.6	-2.9	-4.0
4-hydroxy-3,5-diiodobenzonitrile	3.9	-3.9	-3.9	-5.3
4-hydroxyazobenzene	3.6	-3.3	-3.7	-4.4
4-hydroxybenzoic acid	1.4	-1.4	-0.8	-2.8
4-hydroxyphenylacetic acid	1.0	-0.9	-0.5	-1.7
4-iodobenzoic acid	3.0	-4.0	-3.3	-5.0
4-methoxybenzoic acid	2.0	-2.5	-1.6	-3.1
4-methoxyphenol	1.6	-0.5	-0.6	-1.4
4-methoxyphenylpropionic acid	2.4	-2.2	-1.8	-2.7
4-methylpent-1-ene	3.1	-3.2	-2.5	-2.6
4-methylphenanthrene	4.9	-5.9	-5.4	-4.7
4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline	2.9	-5.8	-6.1	-3.7
4-methylthio-3,5-xylyl methylcarbamate	2.9	-3.9	-3.5	-3.3
4-nitro-5-methylphenol	2.5	-2.1	-1.3	-3.0
4-nitroaniline	1.5	-2.3	-1.6	-2.2
4-nitrotoluene	2.4	-2.5	-2.4	-2.1
4-oxaheptane	2.0	-1.3	-1.7	-1.5
4-tert-butylbenzoic acid	3.8	-3.8	-3.4	-4.7
4-tert-butylphenol	3.4	-2.4	-2.2	-3.7
5'-(trifluoromethanesulphonamide)acet-2',4-xylidide	2.7	-3.2	-3.5	-3.8
5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-	1.7	-2.5	-2.4	-2.5

pyrimidinedione				
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	1.8	-2.5	-2.5	-2.7
5-isopropyl-m-tolyl methylcarbamate	3.2	-3.4	-3.2	-3.3
5-methyl N-(methylcarbamoyloxy)thioacetimidate	0.6	-0.4	-0.5	-0.7
5-methyl-1,2,4-triazolo[3,4-b]benzothiazole	2.5	-2.1	-3.0	-3.6
5-nonanone	2.7	-2.6	-2.9	-2.2
acenaphthene	4.2	-4.6	-3.8	-4.3
acenaphthylene	4.2	-4.0	-3.6	-4.4
acetohexamide	2.4	-2.0	-3.0	-3.6
acetylene	0.5	-1.3	-0.4	0.0
acridine	3.3	-3.7	-4.5	-3.7
adipic acid	0.2	-0.7	0.0	-1.0
aldicarb	1.4	-1.5	-1.5	-1.6
aldoxycarb	-0.7	-1.3	-1.6	0.0
allobarbitiol	1.3	-2.1	-1.1	-2.3
a-methylstyrene	3.4	-3.1	-3.4	-2.9
ametryn	3.3	-3.0	-3.4	-3.4
aminocarb	1.9	-2.4	-2.5	-2.1
amobarbital	2.0	-2.6	-2.3	-2.8
a-naphthol	2.7	-2.2	-2.0	-2.9
a-naphthyl acetate	2.6	-2.6	-3.3	-2.3
aniline	1.1	-0.4	-0.9	-0.6
anthracene	4.4	-6.6	-5.4	-5.8
anthraquinone	3.3	-5.2	-5.8	-5.4
aprobarbital	1.4	-1.7	-1.3	-2.0
atrazine	2.8	-3.8	-3.3	-3.8
azelaic acid	1.7	-1.9	-2.0	-2.0
b(4-chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	3.0	-3.7	-4.2	-3.2
barbital	0.6	-1.4	-1.5	-1.7
bendiocarb	2.6	-2.9	-3.3	-3.1
bendroflumethiazide	1.8	-3.6	-3.8	-3.3
benfluralin	5.3	-6.5	-6.8	-5.2
benzaldehyde	1.7	-1.2	-1.5	-1.2
benzamide	0.7	-1.0	-1.5	-1.3
benzene	2.0	-1.6	-1.8	-1.5
benzidine	1.9	-2.8	-3.9	-2.4
benzimidazole	1.2	-1.8	-2.1	-2.2
benzofluoranthene	6.1	-8.2	-5.5	-6.9
benzoic acid	1.9	-1.6	-1.5	-2.3
benzonitrile	1.5	-1.7	-1.5	-1.0
benzophenone	3.2	-3.1	-3.1	-2.9
benzothiazole	2.2	-1.5	-1.6	-1.7
benzothiophene	3.0	-3.0	-2.4	-2.6
benzotrifluoride	3.0	-3.0	-3.0	-2.5
benzoxazole	1.7	-1.2	-1.8	-1.3
benzyl alcohol	1.1	-0.4	-0.7	-0.6
betamethasone	1.7	-3.8	-3.1	-3.3
betamethasone-17-valerate	3.9	-4.7	-5.5	-5.0
biphenyl	3.8	-4.3	-4.2	-3.7

bis-(4-aminophenyl)methane	2.2	-2.3	-3.7	-2.3
bromobenzene	2.9	-2.5	-2.6	-2.4
bromocyclohexane	3.5	-2.3	-2.6	-2.9
bromomethane	1.2	-0.8	-0.8	-0.7
butacarb	5.0	-4.2	-5.7	-5.3
butalbital	1.9	-2.1	-1.9	-2.5
butanal	0.8	0.0	-0.3	-0.3
butane	2.3	-3.0	-2.0	-1.8
butanoic acid	1.1	-0.2	0.1	-0.6
butocarboxim	1.2	-0.7	-0.6	-0.7
butyl 4-aminobenzoate	2.8	-2.8	-3.1	-2.6
butyl 9-hydroxy-9H-fluorene-9-carboxylate	3.7	-3.9	-3.2	-3.6
butyl acrylate	2.2	-1.8	-2.0	-1.7
butyl alcohol	0.8	-0.1	-0.5	-0.3
butyl benzyl phthalate	4.8	-5.1	-5.1	-4.3
butyl butanoate	2.8	-2.5	-2.5	-2.3
caffeine	0.2	-1.0	-0.8	-1.8
carbaryl	2.4	-3.3	-3.4	-3.1
carbazole	3.2	-5.0	-4.8	-4.9
carbendazim	1.6	-3.8	-2.4	-3.3
carbon tetrabromide	2.8	-3.1	-3.9	-3.0
carbon tetrachloride	2.4	-2.3	-2.8	-1.9
carbon tetrafluoride	1.2	-3.7	-2.2	-0.7
chlorimuron	2.3	-2.5	-4.0	-3.4
chlorobenzene	2.6	-2.4	-2.3	-2.1
chlorocyclohexane	3.4	-2.4	-2.5	-2.9
chlorodifluoromethane	0.9	-1.5	-1.5	-0.4
chloroethane	1.6	-1.0	-1.3	-1.1
chlorothiazide	-0.2	-3.0	-1.7	-2.5
chlorotoluron	2.6	-3.5	-3.1	-3.3
chloroxuron	4.1	-4.9	-5.2	-4.8
chlorpropamide	2.0	-3.0	-2.8	-2.5
chlorsulfuron	2.3	-1.1	-2.0	-3.3
cholesterol	8.7	-6.6	-8.9	-9.5
chrysene	5.5	-8.1	-7.2	-7.4
cinnamic acid	2.1	-2.4	-2.0	-2.7
cis-1,2-dimethylcyclohexane	4.0	-4.3	-3.4	-3.5
cis-1,4-dimethylcyclohexane	4.0	-4.5	-3.4	-3.5
cis-2-butene	2.1	-2.0	-1.5	-1.6
cis-2-hexene	3.1	-3.2	-2.5	-2.6
cis-2-pentene	2.6	-2.5	-2.0	-2.1
cis-crotonic acid	0.9	0.0	0.4	-0.8
coronene	7.3	-9.3	-9.1	-10.9
cortisone	1.8	-3.1	-1.3	-3.3
cortisone acetate	2.1	-4.3	-3.0	-3.7
coumarin	1.5	-1.9	-1.5	-1.4
cyanazine	2.5	-3.2	-3.8	-3.4
cycloate	3.8	-3.4	-3.5	-3.3
cycloheptane	3.7	-3.5	-2.7	-3.2
cycloheptanol	2.1	-0.9	-1.5	-1.6

cycloheptatriene	3.0	-2.2	-2.8	-2.5
cycloheptene	3.5	-3.2	-2.7	-2.9
cyclohexane	3.2	-3.2	-2.1	-2.7
cyclohexanol	1.6	-0.4	-0.8	-1.1
cyclohexanone	1.1	-0.6	-0.8	-0.6
cyclohexene	3.0	-2.6	-2.1	-2.5
cyclooctane	4.2	-4.2	-3.3	-3.7
cyclopentane	2.7	-2.7	-1.4	-2.2
cyclopentene	2.5	-2.1	-1.5	-2.0
cyclopropane	1.7	-2.0	-0.2	-1.2
cyprazine	3.1	-3.5	-3.0	-4.0
dacthal	4.2	-5.8	-5.0	-5.0
daimuron	4.3	-5.3	-5.3	-5.6
decachlorobiphenyl	10.2	-10.8	-12.3	-12.5
decanoic acid	4.0	-3.4	-3.6	-3.6
deoxycorticosterone	3.1	-3.7	-4.1	-3.8
deoxycorticosterone acetate	3.7	-4.6	-4.5	-4.5
desmetryn	2.8	-2.6	-2.3	-2.9
dexamethasone	1.7	-3.8	-3.1	-3.6
diallate	4.1	-4.3	-4.7	-3.6
dibenzodioxin	4.3	-5.3	-5.6	-4.8
dibenzofuran	3.7	-4.7	-4.4	-3.8
dibutyl phthalate	4.6	-4.4	-5.7	-4.1
dichloromethane	1.3	-0.8	-1.2	-0.8
diethyl disulfide	2.9	-2.6	-2.4	-2.4
diethyl ether	1.1	-0.1	-0.6	-0.5
diethyl o-phthalate	2.7	-2.3	-3.1	-2.2
diethyl phthalate	2.7	-2.3	-3.1	-2.1
diethyl sulfide	1.9	-1.5	-2.2	-1.4
diethylstilbestrol	5.6	-4.3	-5.3	-6.6
difenoxuron	3.5	-4.2	-4.8	-4.2
diflubenzuron	3.6	-6.6	-5.4	-5.2
diiodomethane	2.4	-2.5	-2.4	-1.8
diisopropyl ketone	1.6	-1.3	-1.5	-1.1
dimepiperate	4.5	-4.1	-4.2	-4.1
dimetan	1.7	-0.8	-1.4	-1.4
dimethametryn	4.2	-3.7	-3.6	-4.1
dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	-0.3	-0.3	-0.3	-0.1
dimethyl fumarate	1.2	-0.3	0.3	-1.5
dimethyl maleate	1.2	-0.3	0.3	-0.7
dimethyl oxalate	-0.6	-0.3	-1.3	0.8
dimethyl phthalate	1.7	-1.7	-1.8	-1.2
dimethyl sulfide	0.9	-0.5	-1.2	-0.4
dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	4.2	-5.8	-5.0	-5.1
di-n-butyl succinate	3.4	-3.0	-3.0	-2.8
diphenyl ether	4.1	-4.0	-3.8	-3.6
diphenyl phthalate	4.1	-6.6	-6.2	-4.1
diphenylacetic acid	3.1	-3.2	-3.4	-3.8
diphenylamine	3.3	-3.5	-3.5	-3.1
diphenylcarbinol	2.7	-2.5	-2.4	-2.6

diphenylmethane	4.0	-4.1	-4.2	-3.5
dipropalin	4.9	-3.0	-6.2	-5.0
dipropetryn	4.2	-4.2	-3.6	-4.5
diuron	2.7	-3.7	-3.3	-3.5
d-limonene	4.8	-4.0	-4.3	-4.3
dodecane	6.2	-7.7	-6.2	-5.7
dodecanedioic acid	3.2	-3.8	-3.9	-3.7
dodecanol	4.8	-4.7	-5.2	-4.3
E-3-chloro-2-butenoic acid	1.4	-0.6	-0.5	-1.2
estradiol	3.9	-4.8	-4.4	-5.0
estrone	3.4	-4.0	-4.2	-5.3
ethalfluralin	5.2	-6.0	-6.0	-5.1
ethane	1.3	-2.7	-0.9	-0.8
ethiofencarb	2.0	-2.1	-3.1	-1.6
ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	3.2	-4.6	-5.0	-3.7
ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	4.0	-4.4	-5.3	-3.6
ethyl 4-aminobenzoate	1.8	-2.1	-1.8	-1.9
ethyl acetate	0.9	0.0	-0.4	-0.4
ethyl mercaptan	1.3	-0.6	-1.0	-0.8
ethyl N-benzoyl-n-(3,4-dichlorophenyl)-dl-alaninate	4.3	-4.3	-5.1	-4.2
ethyl nitrate	0.5	-0.2	-0.5	0.1
ethyl propyl ether	1.5	-0.7	-1.1	-1.0
ethylbenzene	3.0	-2.8	-2.6	-2.5
ethylcyclohexane	4.1	-4.3	-3.2	-3.6
ethylene	1.3	-2.3	-1.1	-0.8
ethynyl estradiol	4.1	-4.4	-4.1	-5.2
fenobucarb	2.9	-2.7	-3.2	-2.4
fenothiocarb	3.3	-3.9	-4.2	-2.9
fenuron	1.4	-1.6	-1.7	-2.0
flazasulfuron	1.1	-2.3	-3.1	-2.0
flufenoxuron	6.0	-8.1	-9.5	-6.9
flumethiazide	0.1	-0.8	-2.2	-2.3
fluometuron	2.4	-3.3	-3.0	-3.2
fluorene	4.0	-4.9	-4.0	-4.4
fluorobenzene	2.2	-1.8	-1.8	-1.7
fluorotrichloromethane	2.1	-2.1	-2.6	-1.6
forchlorfenuron	2.4	-3.8	-3.7	-3.3
furan	1.4	-0.8	-1.2	-0.9
furfural	0.8	-0.1	-1.1	-0.3
glyburide	4.8	-5.1	-7.4	-5.7
glyceryl triacetate	0.4	-0.6	0.5	0.1
halosulfuron	0.4	-4.5	-2.4	-1.4
heptabarbital	2.8	-3.0	-3.9	-3.8
heptanal	2.3	-2.0	-1.9	-1.8
heptane	3.8	-4.5	-3.5	-3.3
heptanoic acid	2.5	-1.7	-1.6	-2.0
hexachlorobenzene	5.9	-7.7	-6.7	-7.4
hexachloroethane	4.0	-3.7	-4.5	-5.1
hexadecane	8.2	-8.4	-8.3	-7.7
hexaflumuron	5.6	-7.2	-7.6	-6.9

hexafluoroethane	2.2	-4.2	-2.7	-1.7
hexamethylbenzene	5.3	-5.8	-5.5	-6.2
hexanal	1.8	-1.2	-1.3	-1.3
hydrochlorothiazide	-0.1	-2.6	-2.2	-1.9
hydrocinnamic acid	2.3	-1.4	-1.4	-2.0
hydrocortisone	1.6	-3.1	-2.5	-3.0
hydrocortisone-21-acetate	2.4	-4.5	-3.2	-3.8
hydroflumethiazide	0.2	-3.0	-2.7	-2.2
imazosulfuron	1.7	-4.8	-4.1	-2.8
iodomethane	1.6	-1.0	-1.3	-1.1
ipazine	3.9	-3.8	-3.7	-4.0
isobutane	2.2	-3.1	-1.7	-1.7
isobutene	2.2	-2.3	-1.6	-1.7
isonicotinic acid	0.7	-1.4	-0.9	-3.1
isoprocarb	2.4	-2.7	-2.6	-2.6
isopropyl 4,4'-dibromobenzilate	4.9	-6.6	-6.1	-4.9
isopropyl ether	1.9	-1.1	-1.0	-1.4
isopropyl methyl ketone	0.7	-0.2	-0.7	-0.2
isopropyl nitrate	1.7	-1.5	-1.5	-1.2
isopropyl phenylcarbamate	2.7	-3.0	-1.9	-2.8
isopropylbenzene	3.5	-3.3	-3.0	-2.9
isoproturon	2.8	-3.5	-3.0	-3.7
isoquinoline	2.1	-1.5	-2.3	-1.7
isouron	1.5	-2.4	-2.1	-2.0
L-carvone	3.1	-2.1	-3.3	-2.6
linuron	2.9	-3.5	-3.4	-3.1
lufenuron	6.6	-6.9	-9.0	-7.5
m-acetotoluidide	1.7	-2.1	-1.8	-1.6
m-aminophenol	0.2	-0.6	0.2	-0.7
m-benzenedicarboxylic acid	1.8	-3.1	-2.0	-4.5
m-bromobenzoic acid	2.8	-2.7	-2.4	-3.6
m-bromophenol	2.4	-0.9	-1.2	-2.0
m-bromotoluene	3.4	-3.5	-3.0	-2.9
m-chloroaniline	1.7	-1.4	-1.5	-1.2
m-chlorotoluene	3.2	-3.5	-2.8	-2.7
m-cyanoaniline	1.2	-1.2	-1.1	-1.0
m-cymene	4.0	-3.5	-3.5	-3.5
m-diethylbenzene	4.1	-3.7	-3.6	-3.6
mebendazole	2.7	-3.6	-4.1	-4.8
methabenzthiazuron	2.7	-3.6	-3.4	-3.1
methanethiol	0.8	-0.5	-0.5	-0.3
methiocarb	2.9	-3.9	-3.5	-3.3
methomyl	0.6	-0.4	-0.5	-0.6
methoxybenzene	2.1	-2.0	-1.8	-1.6
methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	4.5	-5.6	-5.8	-4.2
methyl 2,4-dichlorophenoxyacetate	2.9	-3.0	-2.5	-2.6
methyl 3-m-tolylcarbamoyloxyphenylcarbamate	3.3	-4.8	-4.9	-4.0
methyl 4-aminobenzoate	1.3	-1.6	-1.2	-1.7
methyl 4-hydroxybenzoate	2.0	-1.8	-0.6	-2.5
methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	4.2	-5.9	-6.1	-4.3

methyl acrylate	0.7	-0.2	-0.4	-0.2
methyl benzoate	1.8	-1.8	-1.7	-1.3
methyl chloride	1.1	-1.0	-0.7	-0.6
methyl isopropyl ether	1.0	-0.1	-0.3	-0.5
methyl methacrylate	1.3	-0.8	-1.2	-0.8
methyl n-butyl ether	1.5	-1.0	-1.1	-1.0
methyl propyl ether	1.1	-0.4	-0.6	-0.5
methyl tert-butyl ether	1.4	-0.2	-0.7	-0.9
methylcyclohexane	3.6	-3.8	-2.7	-3.1
methylcyclopentane	3.1	-3.3	-2.1	-2.6
methyldymron	3.6	-3.3	-5.1	-3.6
methylphenylsulfide	2.6	-2.4	-2.4	-2.1
methylprednisolone	1.8	-3.5	-2.7	-3.5
metobromuron	2.5	-2.9	-3.0	-2.7
metolcarb	1.7	-1.8	-1.9	-1.7
Metoxuron	2.1	-2.5	-2.9	-2.6
m-fluorobenzoic acid	2.1	-2.0	-1.4	-2.6
m-hydroxybenzaldehyde	1.2	-1.2	-0.5	-1.6
m-hydroxybenzyl alcohol	0.6	-0.3	0.3	-0.6
m-hydroxytoluene	2.1	-0.7	-0.7	-1.6
m-nitrobenzaldehyde	1.5	-2.0	-1.9	-1.4
m-nitrobenzoic acid	1.7	-1.7	-1.9	-2.4
m-nitrobenzyl alcohol	0.9	-2.4	-1.1	-0.4
m-nitrobromobenzene	2.7	-1.3	-2.7	-2.5
m-nitrophenol	1.9	-1.0	-0.7	-2.1
monuron	2.0	-2.9	-2.5	-3.0
m-terphenyl	5.5	-5.2	-6.8	-5.6
m-toluic acid	2.4	-2.1	-1.8	-2.8
m-toluidine	1.6	-0.9	-1.4	-1.1
m-xylene	3.1	-2.8	-2.6	-2.6
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	4.8	-6.0	-5.3	-4.6
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine	5.1	-5.6	-7.0	-4.8
N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	4.0	-5.5	-5.4	-4.2
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	3.3	-4.4	-3.1	-3.8
N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea	2.1	-2.5	-2.9	-2.6
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	4.2	-4.5	-4.6	-4.2
N-(4-chlorophenyl)-2,2-dimethylpentanamide	4.1	-4.0	-4.5	-4.2
N'-(4-chlorophenyl)-N-methoxy-N-methylurea	2.3	-2.4	-2.6	-2.3
N-(cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl)benzenamine	5.6	-6.5	-5.2	-5.2
N,N'-(2-hydroxyethyl)-1,4-diaminoanthraquinone	2.7	-5.8	-6.6	-4.4
N,N-(2-hydroxyethyl)-4-phenylazoaniline	2.8	-4.0	-4.6	-3.3
N,N-diethyl-2-(1-naphthyloxy)propionamide	3.3	-3.6	-3.9	-3.3
N,N-dimethyl-2,2-diphenylacetamide	2.9	-3.0	-2.5	-3.4
N,N-dimethyl-4-phenylazoaniline	4.3	-6.0	-4.7	-4.7
N,N-dimethylaniline	2.2	-1.9	-2.1	-1.7
N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea	2.4	-3.3	-3.5	-3.2
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea	2.8	-3.5	-3.0	-3.7
N,N'-dinitroethanediamine	-1.8	-1.8	-1.5	0.8

N,N'-di-n-propyladipamide	1.2	-1.8	-3.0	-2.2
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	3.4	-5.4	-4.6	-4.3
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-propanamide (sufentanil)	3.6	-3.7	-4.9	-3.8
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea	1.8	-2.0	-2.0	-2.7
naphthalene	3.2	-3.6	-3.4	-3.2
n-butyl mercaptan	2.3	-2.2	-2.1	-1.7
n-butylbenzene	4.0	-4.1	-3.7	-3.5
N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea	4.2	-4.8	-5.3	-4.4
N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline	5.3	-6.5	-5.8	-5.2
n-decane	5.3	-6.4	-5.1	-4.7
n-hexane	3.3	-4.0	-3.0	-2.8
nicosulfuron	-1.2	-1.5	-1.1	0.5
nicotinic acid	0.7	-0.8	-0.6	-2.3
nitralin	2.9	-5.8	-6.3	-3.7
nitrobenzene	1.8	-1.8	-1.8	-1.3
nitroethane	0.5	-0.2	-0.5	0.1
N-methyl-2,4,6,N-tetranitroaniline	1.6	-3.6	-4.9	-2.2
n-octane	4.3	-5.2	-4.1	-3.8
n-octylbenzene	6.0	-6.5	-5.8	-5.5
nonanal	3.3	-3.2	-2.9	-2.8
nonane	4.8	-6.0	-4.6	-4.3
nonanoic acid	3.5	-2.7	-2.9	-3.0
norethindrone	3.0	-4.6	-3.7	-4.3
norethindrone acetate	4.0	-4.8	-4.9	-5.3
novaluron	5.3	-7.0	-6.7	-6.3
n-pentadecane	7.7	-9.4	-7.7	-7.2
N-phenyl-N[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)	3.9	-3.2	-5.7	-4.0
n-propylbenzene	3.5	-3.4	-3.2	-3.0
N-Sulfanilylsulfanilamide	0.1	-2.8	-2.4	-0.7
N-tert-butylurea	0.3	-0.7	-0.4	-1.3
n-tridecane	6.7	-7.6	-6.7	-6.2
n-undecane	5.7	-7.6	-5.6	-5.2
O-(2-chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate	3.4	-4.3	-4.4	-3.1
O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate	5.1	-6.1	-5.7	-4.9
O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphonothioate	6.3	-7.1	-6.5	-6.3
O,O-diethyl O-4-nitrophenyl phosphorothioate	3.7	-4.4	-4.9	-3.2
O,O-diethyl O-quinoxalin-2-yl phosphothioate	3.0	-4.1	-4.9	-2.6
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	4.7	-5.5	-5.9	-4.3
O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	4.1	-4.2	-4.9	-3.7
O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	4.9	-5.5	-5.3	-4.5
O,O-dimethyl O-4-nitrophenyl phosphorothioate	2.8	-3.8	-3.5	-2.4
O,O-dimethyl S-[2-(methylamino)-2-oxoethyl]	0.3	-1.0	-0.4	0.0

phosphorodithioate				
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	3.7	-4.8	-4.6	-3.4
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl O,O-diethyl phosphorothioate	3.5	-4.9	-5.9	-3.3
o-acetoxybenzoic acid	1.1	-1.6	-1.4	-1.7
o-aminophenol	0.6	-0.7	0.6	-1.6
o-benzenedicarboxylic acid	1.1	-1.4	-2.7	-2.7
o-bromobenzoic acid	2.4	-2.0	-2.5	-3.2
o-bromobenzyl alcohol	2.0	-2.2	-1.8	-2.0
o-chloroacetanilide	1.2	-1.4	-0.9	-1.3
o-chloroaniline	1.7	-1.2	-1.3	-1.2
o-chloroanisole	2.7	-2.5	-2.4	-2.2
o-chlorotoluene	3.2	-2.5	-2.8	-2.7
octafluoropropane	3.1	-4.5	-3.4	-2.6
octanal	2.8	-2.4	-2.4	-2.3
octanoic acid	3.0	-2.3	-2.3	-2.5
o-cymene	4.0	-3.8	-3.5	-3.5
o-diethylbenzene	4.1	-3.3	-3.6	-3.6
O-ethyl O-(4-nitrophenyl)phenylphosphonothioate	4.5	-5.0	-4.7	-4.1
o-ethyltoluene	3.6	-3.2	-3.1	-3.1
o-fluorobenzoic acid	1.7	-1.3	-1.4	-2.3
o-hydroxyacetanilide	0.6	-2.2	-0.6	-0.8
o-hydroxybenzamide	1.0	-1.8	-0.8	-1.7
o-hydroxybenzyl alcohol	0.6	-0.3	0.2	-0.7
o-hydroxybiphenyl	3.3	-2.4	-2.8	-3.1
o-hydroxytoluene	2.1	-0.6	-0.7	-1.6
o-methoxybenzamide	0.3	-1.8	-1.9	-0.8
o-methoxybenzoic acid	1.6	-1.5	-1.8	-1.9
o-methoxyphenol	1.3	-0.8	-0.4	-0.9
o-nitroacetanilide	1.1	-1.9	-1.9	-1.3
o-nitrobenzaldehyde	1.5	-1.8	-2.0	-1.2
o-nitrobenzoic acid	1.4	-1.3	-2.3	-2.1
o-nitrobenzyl alcohol	0.9	-1.5	-1.5	-0.9
o-nitrophenol	1.9	-1.7	-0.7	-1.6
o-nitrotoluene	2.4	-2.3	-2.3	-1.9
o-phenylenediamine	0.2	-0.4	-0.8	-0.4
o-terphenyl	5.5	-5.3	-6.3	-5.3
o-toluic acid	2.1	-2.1	-1.8	-2.4
o-toluidine	1.6	-0.8	-1.4	-1.1
o-tolylurea	1.3	-1.8	-1.2	-2.4
oxasulfuron	1.3	-3.9	-3.8	-2.1
o-xylene	3.1	-3.0	-2.6	-2.6
p-acetotoluidide	1.7	-2.1	-1.8	-2.4
p-aminobenzene sulphonamide	-0.6	-1.4	0.1	-0.4
p-aminophenol	0.2	-1.3	-0.1	-1.4
p-benzoquinone	0.3	-1.0	-1.7	-0.6
p-bromobenzoic acid	2.8	-3.5	-2.7	-4.5
p-bromobenzyl alcohol	2.0	-2.2	-1.6	-2.0
p-bromophenyl urea	1.6	-1.6	-1.9	-3.1
p-bromotoluene	3.4	-3.2	-3.0	-3.0

p-chloroacetanilide	1.7	-2.8	-2.0	-2.8
p-chloroaniline	1.7	-1.5	-1.7	-1.7
p-chlorotoluene	3.2	-3.1	-2.8	-2.7
p-cyanobenzoic acid	1.4	-2.1	-2.0	-2.9
p-cymene	4.0	-3.8	-3.5	-3.5
p-diethylbenzene	4.1	-3.6	-3.6	-3.6
p-difluorobenzene	2.4	-2.0	-2.0	-1.9
pebulate	3.5	-3.3	-3.8	-3.0
penbutolol	4.2	-1.6	-2.8	-4.2
Pencycuron	5.5	-6.0	-6.7	-6.1
Pendimethalin	4.8	-6.0	-6.2	-4.6
pentachlorobenzene	5.2	-5.5	-5.1	-5.3
pentachloronitrobenzene	5.0	-5.8	-5.5	-5.7
pentachlorophenol	4.7	-4.3	-3.9	-5.9
pentaerythrityl tetrabromide	4.1	-5.4	-5.3	-4.9
pentafluorochloroethane	2.5	-3.4	-2.8	-2.0
pentamethylbenzene	4.7	-4.0	-4.1	-4.5
pentane	2.8	-3.3	-2.5	-2.3
pentanoic acid	1.6	-0.6	-0.4	-1.1
pentyl 4-aminobenzoate	3.3	-3.3	-3.8	-3.0
perylene	6.1	-8.8	-7.8	-8.1
p-ethoxyacetanilide	1.7	-2.4	-2.2	-2.3
p-ethyl hydroxybenzoate	2.5	-2.3	-1.2	-2.9
p-ethylphenol	2.6	-1.4	-1.3	-2.3
p-ethyltoluene	3.6	-3.2	-3.3	-3.1
p-fluorobenzoic acid	2.1	-2.1	-1.7	-3.2
phenanthrene	4.4	-5.2	-5.1	-4.6
phenanthridine	3.3	-2.8	-4.2	-3.6
Phenobenzuron	3.0	-4.3	-6.2	-3.4
phenol	1.5	-0.1	-0.3	-1.2
phenolphthalein	3.1	-5.2	-5.1	-4.9
phenyl glycidyl ether	1.6	-1.8	-1.6	-1.1
phthalazine	1.1	-0.4	-2.0	-1.3
p-hydroxybenzyl alcohol	0.6	-1.3	0.3	-1.1
p-hydroxytoluene	2.1	-0.7	-0.9	-1.7
picric acid	1.5	-1.3	-2.2	-2.0
pimilic acid	0.7	-0.5	-0.6	-1.0
pirimicarb	1.4	-1.9	-0.6	-1.6
p-isopropylbenzoic acid	3.3	-3.0	-2.7	-3.8
p-methoxyacetanilide	1.2	-1.0	-1.6	-1.7
p-methoxybenzaldehyde	1.8	-1.5	-1.8	-1.3
p-methoxyphenol	1.6	-0.5	-0.6	-1.4
p-methylbenzyl alcohol	1.6	-1.2	-1.2	-1.5
p-nitroacetanilide	1.6	-1.9	-1.9	-3.1
p-nitrobenzaldehyde	1.5	-1.8	-2.2	-1.8
p-nitrobenzoic acid	1.7	-2.9	-2.2	-3.3
p-nitrobenzyl alcohol	0.9	-1.9	-1.1	-1.1
p-nitrophenol	1.9	-1.1	-1.0	-2.3
p-N-methylhydroxyaniline	0.8	-1.1	-0.9	-0.9
p-phenylazoaniline	3.2	-3.8	-4.2	-3.7

p-phenylenediamine	-0.4	-0.5	-1.0	-0.3
p-propylphenol	3.0	-2.0	-1.8	-2.5
prasterone	3.0	-3.7	-3.9	-3.7
prasterone acetate	4.0	-4.5	-4.9	-4.9
prednisolone	1.4	-3.2	-2.2	-3.0
prednisone	1.6	-3.5	-2.2	-3.2
pregnenolone	3.9	-4.7	-5.2	-5.1
prodiamine	4.9	-7.4	-6.7	-5.4
profluralin	5.6	-6.5	-6.5	-5.2
progesterone	3.7	-4.6	-5.0	-4.2
promecarb	3.2	-3.4	-3.2	-3.3
prometon	3.6	-2.5	-2.5	-3.7
prometryn	3.7	-3.9	-3.7	-4.2
propane	1.8	-2.8	-1.4	-1.3
propazine	3.2	-4.4	-3.2	-4.6
propene	1.7	-2.3	-1.3	-1.2
propoxur	1.9	-2.1	-2.3	-2.0
propyl 4-aminobenzoate	2.3	-2.3	-2.5	-2.3
propyl 4-hydroxybenzoate	3.0	-2.6	-1.9	-3.2
propylcyclopentane	4.1	-4.7	-3.1	-3.6
p-terphenyl	5.5	-7.1	-7.1	-6.9
p-toluic acid	2.4	-2.6	-2.1	-3.5
p-toluidine	1.6	-1.2	-1.5	-1.3
p-xylene	3.1	-2.8	-2.6	-2.6
pyrazosulfuron-ethyl	0.3	-4.5	-3.1	-1.3
pyrene	4.9	-6.2	-5.8	-5.7
pyrrole	0.9	-0.2	-0.7	-0.4
quinoline	2.1	-1.3	-2.3	-1.6
rimsulfuron	0.0	-4.6	-2.6	-1.1
S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate	3.5	-4.5	-5.0	-3.3
S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethyl phoshorodithioate	2.5	-4.2	-3.7	-2.5
S-2,3,3-trichloroallyl diisopropylthiocarbamate	4.6	-4.9	-4.5	-4.2
sebacic acid	2.2	-2.3	-2.6	-2.7
secbumeton	3.6	-2.6	-2.5	-3.8
sec-butylbenzene	4.0	-3.8	-3.5	-3.5
siduron	3.9	-4.1	-4.1	-4.5
simazine	2.4	-4.5	-3.4	-3.9
simetryn	2.9	-2.7	-3.1	-3.0
beta-naphthol	2.7	-2.3	-2.0	-3.1
styrene	2.9	-2.5	-2.6	-2.4
suberic acid	1.2	-1.2	-1.3	-1.9
succinic acid	-0.8	-0.2	1.3	-0.3
sulfabenzamide	1.3	-3.0	-3.2	-2.4
sulfacetamide	-0.6	-1.2	-1.0	-0.5
sulfacytine	-0.7	-2.2	-2.1	-0.2
sulfadiazine	-0.3	-3.5	-2.0	-1.5
sulfadimethoxine	1.2	-3.0	-2.8	-2.4
sulfaethidole	0.9	-1.9	-2.3	-2.0
sulfamerazine	0.2	-3.1	-2.6	-1.8

sulfameter	-0.3	-2.6	-2.0	-1.1
sulfamethazine	0.8	-2.3	-3.2	-1.8
sulfamethizole	0.4	-2.4	-2.0	-1.7
sulfamethomidine	0.8	-2.5	-3.5	-1.5
sulfamethoxazole	0.5	-2.6	-2.1	-1.4
sulfamethoxypyridazine	0.2	-3.3	-2.5	-1.3
sulfamethylthiazole	1.3	-2.1	-2.6	-2.9
sulfamoxole	1.0	-2.2	-3.1	-2.2
sulfaperine	0.2	-2.8	-2.6	-2.1
sulfapyrazine	-0.3	-3.7	-2.0	-1.4
sulfapyridine	0.5	-3.0	-2.6	-1.7
sulfaquinoxaline	0.8	-4.6	-4.0	-2.6
sulfathiazole	0.7	-2.8	-1.9	-2.0
sulfisomidine	0.8	-2.2	-3.2	-2.4
sulfisoxazole	1.0	-2.9	-2.7	-2.2
sulfometuron-methyl	1.7	-3.2	-3.3	-3.0
sulfosulfuron	1.0	-4.4	-4.1	-2.3
tebuthiuron	1.8	-2.0	-2.0	-2.7
teflubenzuron	4.6	-7.3	-6.6	-6.1
terbumeton	3.6	-3.2	-3.3	-4.1
terbuthylazine	3.3	-4.4	-4.7	-4.3
terbutryn	3.8	-4.0	-4.4	-4.1
tert-butyl bromide	2.5	-2.4	-2.0	-2.0
tert-butyl chloride	2.5	-1.5	-1.9	-1.9
tert-butylbenzene	3.9	-3.7	-3.3	-3.4
testosterone	3.3	-4.1	-3.9	-4.1
testosterone acetate	4.3	-5.2	-5.0	-4.9
testosterone propionate	4.8	-5.4	-5.1	-5.2
tetrachloroethene	3.0	-2.9	-3.1	-2.5
tetradecane	7.2	-8.0	-7.2	-6.7
tetrafluoroethylene	1.2	-2.8	-1.2	-0.7
tetramethysuccinic acid	1.0	-1.6	-0.6	-2.1
theophylline	-0.4	-1.4	-0.3	-1.6
thiazafluron	0.8	-2.1	-1.1	-1.5
thiobencarb	3.9	-4.0	-4.2	-3.4
thiofanox	2.2	-1.6	-1.8	-2.0
thiophene	1.8	-1.4	-1.0	-1.3
thymine	-0.3	-1.5	0.4	0.6
thymol	3.5	-2.2	-2.1	-3.3
tolbutamide	2.4	-3.4	-3.3	-2.9
toluene	2.5	-2.2	-2.1	-2.0
trans-1,2-dimethylcyclohexane	4.0	-4.3	-3.4	-3.5
trans-1,4-dimethylcyclohexane	4.0	-4.5	-3.4	-3.5
trans-2-butene	2.1	-2.0	-1.5	-1.6
trans-2-pentene	2.6	-2.5	-2.0	-2.1
trans-azobenzene	4.1	-4.5	-4.7	-4.0
triamcinolone	1.0	-3.7	-2.2	-2.9
triamcinolone diacetate	1.5	-4.1	-3.5	-3.1
triasulfuron	2.4	-4.1	-3.9	-3.5
tribromomethane	1.8	-1.9	-2.1	-1.3

trichlormethiazide	0.2	-2.7	-3.8	-2.2
trichloroacetic acid	1.4	-0.6	-0.6	-1.3
trichloroethylene	2.5	-2.0	-2.4	-2.0
trichloromethane	1.5	-1.2	-1.8	-1.0
tridecanoic acid	5.5	-3.8	-5.4	-5.2
trietazine	3.4	-4.1	-4.2	-3.7
triflumuron	4.2	-7.2	-6.5	-5.4
trifluoromethane	0.6	-1.2	-1.4	-0.1
trifluralin	5.3	-6.3	-6.8	-5.0
trinitroglycerine	1.5	-2.2	-2.1	-1.0
triphenylene	5.5	-6.7	-7.7	-6.7
undecanedioic acid	2.7	-1.6	-3.3	-3.0
undecanoic acid	4.5	-3.6	-4.2	-4.0
vinyl acetate	0.7	-0.6	-0.5	-0.2
vinyl chloride	1.6	-0.9	-1.4	-1.1
XMC	2.3	-2.6	-2.5	-2.5
xylylcarb	2.3	-2.5	-2.5	-2.3
Z-3-chloro-2-butenoic acid	1.4	-0.6	-0.5	-1.5

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