ESTIMATION OF MELTING POINTS OF ORGANIC COMPOUNDS

By

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AKASH JAIN

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DEDICATION

To my parents and Bhumika

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ABSTRACT

Melting point finds applications in chemical identification, purification and in the calculation of a number of other physicochemical properties such as vapor pressure and aqueous solubility. Despite the availability of enormous amounts of experimental data, no generally applicable methods have been developed to estimate the melting point of a compound from its chemical structure. A quick estimation of melting point can be a useful tool in the design of new chemical entities.

In this dissertation, a simple means of estimating the melting points for a large variety of pharmaceutically and environmentally relevant organic compounds is developed. Melting points are predicted from the separate calculation of the enthalpy and entropy of melting directly from the chemical structure. The entropy of melting is calculated using a semi-empirical equation based on only two non-additive molecular parameters. This equation is validated and refined using a large collection of experimental entropy of melting values. The enthalpy of melting is calculated by additive group contributions.

Melting points are estimated from the ratio of the enthalpy of melting and the entropy of melting. All of the methods and group contributions developed in this study are compatible with the UPPER (Unified Physical Property Estimating Relationships) scheme. The predicted melting points are compared to experimental melting points for over 2200 organic compounds collected from the literature. The average absolute error in melting point prediction is 30.1 °. This is a very reasonable estimate considering the size and diversity of the dataset used in this study.

CHAPTER 1: INTRODUCTION

Melting point is of great importance in the calculation of several physicochemical properties. As seen in figure 1.1, melting point (T_m) is an integral part of Yalkowsky's UPPER scheme (Yalkowsky et al., 1994).

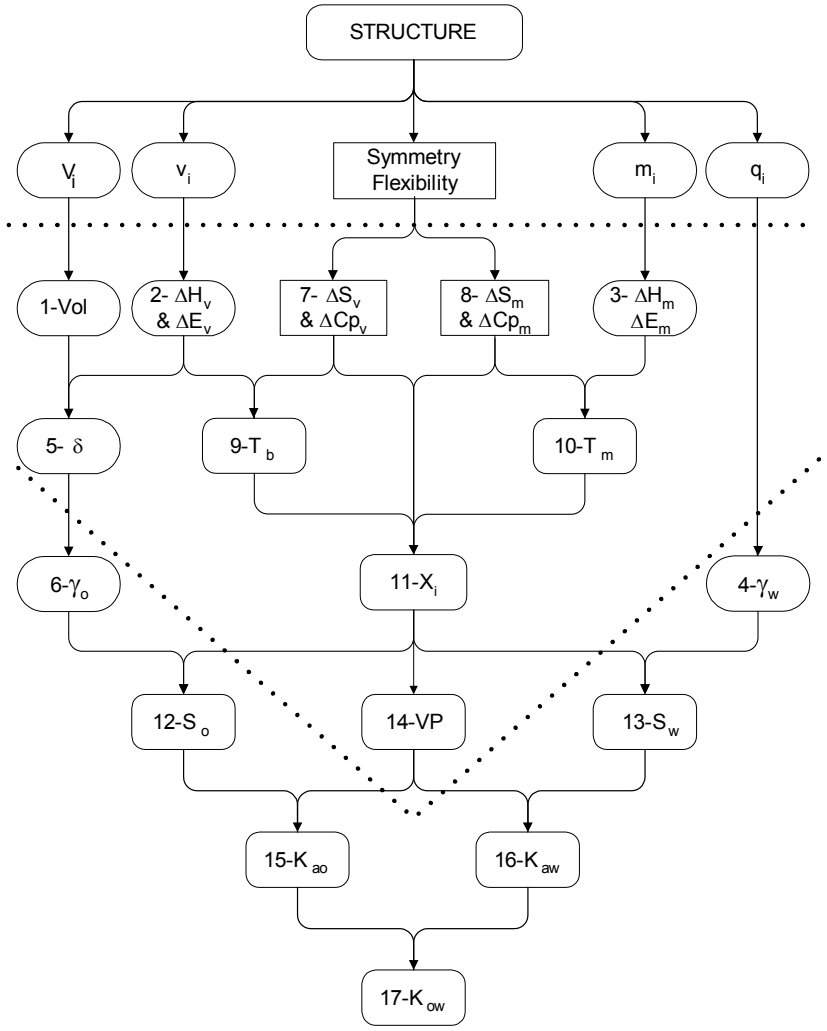


Figure 1.1. UPPER (Unified Physical Property Estimation Relationships) Scheme

T_m is used in the estimation of ideal crystalline solubility (X_i) which in turn is used to calculate octanol solubility (S_o), vapor pressure (VP) and aqueous solubility (S_w). T_m is used as a descriptor for properties like aqueous solubility (Yalkowsky, 1981, Jain et al., 2001, Ran et al., 2001), vapor pressure (Katritzky et al., 2001), liquid viscosity (Nikmo et al., 2002) and behavior of eutectic compositions (Law et al., 2002).

Melting point is useful in pre-formulation studies for characterization and screening of drugs. Melting point has great significance in the field of environmental science as well. It indicates the physical state of a chemical at ambient temperatures and provides valuable information regarding its handling and treatment. Because of its relationship with vapor pressure and aqueous solubility, melting point is an important property for understanding the absorption, distribution and transport of chemicals in the environment (Dearden, 2003) as well as in the human body.

Unfortunately, there are few models available for predicting melting point, and compounds have to be synthesized and their melting points experimentally measured before any other properties are predicted. Often there are problems of thermal instability involved in the measurement. Although a large number of experimental melting points are available, often there are chemicals released into the environment which have no reported melting points. In addition, there are always new chemical entities submitted to regulatory agencies without any experimental data (Dearden, 2003). In an attempt to minimize the above mentioned problems, the development of a simple, accurate and widely applicable prediction model for melting points of organic compounds is desired.

Although melting point is the most widely reported property for organic compounds, its relationship to chemical structure is not clearly understood. Despite the availability of vast amounts of experimental melting point data, there is no general relationship relating melting point directly to chemical structure. Melting points, although analogous to boiling points, are more difficult to predict. Boiling points generally show a regular increase within homologous series and are nearly identical for isomers. However, the experimental data in Table 1.1 suggest that melting points do not show a regular increase with homologation. Also the melting points of alkyl isomers (Table 1.2), isomeric arenes (Table 1.3) and disubstituted benzenes (Table 1.4) are widely different and irregular. As a result, no group contribution schemes are capable of adequately predicting melting points, even for simple molecules.

Table 1.1. Experimental melting points (°C) of some homologous series

Alkyl Chain length	Alkanes	Alkanols	Alkanoic Acids
1	-183	-98	8
2	-184	-114	26
3	-188	-124	-20
4	-138	-88	-8
5	-130	-77	-34
6	-95	-47	-3
7	-90	-33	-7
8	-57	-15	17
9	-53	-8	12
10	-30	6	31
11	-9	25	29
12	6	40	54
13	18	50	62
14	28	61	69

Table 1.2. Experimental melting points for some octanes

Compound	Melting Point (°C)
n-octane	-56
2-methylheptane	-109
3-methylheptane	-120
4-methylheptane	-121
2,2-dimethylhexane	-121
2,5-dimethylhexane	-91
3,3-dimethylhexane	-126
2,2,3-trimethylpentane	-113
2,2,4-trimethylpentane	-107
2,3,3-trimethylpentane	-109
2,3,4-trimethylpentane	-109
2,2,3,3-tetramethylbutane	101

Table 1.3. Experimental melting points for isomeric arenes

Compound	Melting Point (°C)
o-xylene	-25
m-xylene	-48
p-xylene	13
hexylbenzene	-62
p-diisopropylbenzene	-17
s-triethylbenzene	-66
hexamethylbenzene	166
anthracene	216
phenanthrene	101
1,2-benzanthracene	162
2,3-benzanthracene	335
3,4-benzphenanthrene	168
2,3-benzphenanthrene	254
9.10-benzphenanthrene	199

Table 1.4. Experimental melting points (°C) for some disubstituted benzenes

Substituent	CH3	Cl	Br	I	NO_2	OCH_3
1,2-di-	-25	-17	-30	-31	118	-37
1,3-di-	-47	-24	84	40	90	22
1,4-di-	13	53	106	131	174	56

A number of methods are currently available for estimating melting points. These methods are either based on group contributions (Joback et al., 1987, Simmamora et al., 1994, Krzyzaniak et al., 1995, Austin, 1930, Constantinou and Gani, 1994, Marrero and Gani, 2001) or physical and structural molecular parameters like molecular cohesiveness, bulkiness, hydrogen-bonding parameters and geometric factors (Kier et al., 1976, Dearden et al., 1988, Abramowitz et al., 1990). Although these methods are reasonably accurate, they are limited in their application as they are based on small datasets of simple molecules and/or homologous series. The group contribution schemes, as described earlier, cannot distinguish between isomers and are incapable of accounting for the geometric properties that influence the process of melting.

The goal of this dissertation is to develop a simple, accurate and widely applicable model for predicting melting points of organic compounds directly from chemical structure. The model is a combination of additive group contributions and non-additive molecular parameters which take into account the anomalies in experimental melting points of isomers and homologous series. In order to develop such a model, the following objectives are defined:

1. A reliable database of experimental values
2. A sound thermodynamic relationship with minimum number of assumptions
3. A reasonable molecular fragmentation pattern based upon a single molecular structure descriptor such as the SMILES string

4. Ability to characterize molecular properties that are not strictly additive and constitutive, and to distinguish between isomers
5. Validation of the model on a wide range of simple structures

The UPPER-based estimation model is based on a fundamental thermodynamic relationship for phase transition. For a phase transition at equilibrium, the free energy change is equal to zero. The melting point is therefore related to the enthalpy (ΔH_m) and entropy of melting (ΔS_m) by the following relationship:

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

The calculations of each of these properties are described in the following chapters.

Chapter 2 defines the enthalpy of melting. The enthalpy of melting is shown to be group-additive. A novel molecular fragmentation scheme for calculating the enthalpy of melting is developed. The scheme is based on SMILES string notations. The wide application of the scheme is discussed as it applies to complex structures of drug-like molecules, herbicides and pesticides. Proximity factors included in the fragmentation scheme are discussed. A tabulation of the various molecular fragments and proximity factors present in the database is provided.

Chapter 3 deals with the entropy of melting. The semi-empirical equation of Dannenfelser et al. (1996, 1999) for entropy of melting is revisited and refined. The non-additive molecular parameters, rotational symmetry and flexibility, that constitute the

entropy of melting are discussed in detail. Methods for calculating each of these parameters are described.

Chapter 4 is based on the estimation of melting points from the combination of enthalpy and entropy of melting. The errors in melting point estimation are carefully evaluated. The prediction ability of the model is assessed using cross-validation.

In Chapter 5, the developed model is compared to an existing computer program that calculates melting points directly from SMILES string input. It is shown that our model provides more accurate estimations of melting points for over 2200 organic compounds.

CHAPTER 2: ENTHALPY OF MELTING

INTRODUCTION

The heat required to melt one mole of a solid is the enthalpy of melting. It is the difference between the enthalpy of the solid and liquid phases. In the solid, as in the liquid, each molecular fragment contributes to dispersion, induction, dipolar, and hydrogen bonding interactions and the total intermolecular interaction energy is the sum of all the pair-wise group interactions. The enthalpy of melting can, therefore, be estimated by additive group contributions.

Group contributions are the simplest methods for estimating the enthalpy of melting. A number of group contribution methods are well documented in the literature (Joback et al. 1987, Chickos et al. 1989, Constantinou et al. 1994, Marrero et al. 2001). Joback et al. developed a first-order group contribution with 40 groups for organic compounds that may contain halogens, oxygen, nitrogen, and sulfur. The group contribution values were obtained from a small dataset of 155 compounds and the average absolute error in enthalpy of melting estimation was 2.03 kJ/mol. Chickos et al. (1989) estimated the enthalpies of melting for 191 hydrocarbons using a group contribution with 20 structural parameters. The average deviation for this method was 2.34 kJ/mol. Constantinou et al. developed a two-tier group contribution scheme containing 63 first-order groups and 40 second –order groups. While the first-order groups included the smaller, simpler groups, the second-order groups accounted for the proximity effects and to distinguish between

the isomers. In order to include more complex structures in their scheme, Marrero and Gani (2001) developed a three-level group contribution scheme. The third level groups account for complex heterocyclic and large polyfunctional alicyclic compounds. Based on a dataset of 686 compounds, they obtained an average absolute error of 3.60 kJ/mol. Although the above mentioned methods have sufficient accuracy, they are either based on small, restricted datasets or consist of complex multi-level calculations that take more time and effort to use.

Another method for estimating the enthalpy of melting is from the product of the melting points and entropies of melting (Kirshenbaum, 1965, Chickos et al. 1999). This method was used mainly for estimating enthalpies of melting for homologous series and polymers. It is also useful for the generation of enthalpy data for compounds with no reported enthalpy values in the literature (Chickos et al. 2002).

In our model, the enthalpy of melting is estimated by a group contribution scheme. The scheme is developed from a large, structurally complex database of over 2200 organic compounds. Mathematically, the scheme can be written as

$$\Delta H_m = \sum n_i m_i + \sum n_j m_j \qquad (2.1)$$

Where

n_i = number of times that group *i* appears in a compound

n_j = number of times that proximity factor *j* appears in a compound

m_i = contribution of group *i* to the enthalpy of melting (kJ/mol)

m_j = contribution of proximity factor *j* to the enthalpy of melting (kJ/mol)

In the UPPER scheme (Figure 1.1), the melting points are usually not known and they are calculated from the enthalpy of melting and not vice-versa. Therefore, enthalpy of melting cannot be estimated using the entropy of melting and melting points. The estimation using group contributions helps maintain the integrity of the UPPER scheme. This method is also useful in cases where melting temperature and entropy of melting data are unavailable.

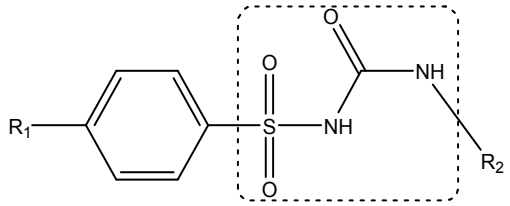
DATA

For the development of a group contribution scheme, experimental melting points, and entropies of melting were collected from the literature. The majority of the experimental melting points and all of the entropy values were obtained from Chickos et al., 1999. Melting points for disubstituted benzenes were obtained from Katritzky et al., 1997. Melting points for drugs, herbicides and steroids were obtained from the electronic and print literature (Merck Index, 1996, Howard et al., 1997, Chickos et al., 2002, Chemfinder, 2004, MPBPWIN v 1.41). Compounds not included in the database are the polyalicyclic cage-like compounds such as adamantane, and compounds with reported enthalpy or entropy values that are less than 1.0 kJ/mol or 8.0 J/K.mol respectively.

MODEL

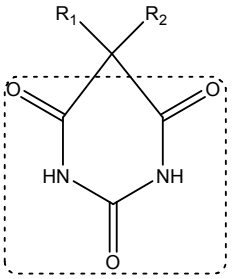
Group Definition

The molecular fragmentation scheme for calculating the enthalpy of melting is based on the concept of an isolating carbon. This concept was introduced by Hansch (1979) and has been successfully used in the fragmentation scheme of ClogP (Leo, 1993). An isolating carbon is a carbon that is not doubly or triply bonded to a hetero-atom. Each molecular fragment is defined as 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. The use of this concept allows us to identify a wide array of molecular fragments ranging from single atoms to large polyatomic groups. For example, single atoms like C, N, O and small functionalities like $–CH_3$ and $-NH_2$ are defined as individual groups. Fragments like $>SO_2NHC(=O)NH-$ of the sulfonylureas and $-C(=O)NHC(=O)NHC(=O)-$ of the barbiturates are also individual groups because there are no isolating carbons in these fragments, as seen in figures 2.1(a) and 2.1(b). Based on this definition, 128 groups are identified in this dataset of 2230 compounds.



Sulfonylurea	R_1	R_2
Tolazamide	CH_3	$C_6H_{12}N$
Acetohexamide	$C(=O)CH_3$	C_6H_{11}
Tolbutamide	CH_3	$(CH_2)_3CH_3$
Chlorpropamide	Cl	$CH_2CH_2CH_3$

Figure 2.1(a). Sulfonylureas



Barbiturate	R_1	R_2
Amobarbital	C_2H_5	$(CH_3)_2CHCH_2CH_2$
Aprobarbital	$CH_2=CHCH_2$	$(CH_3)_2CH$
Butabarbital	C_2H_5	$CH_3CH_2CH(CH_3)$
Butalbital	$CH_2CH=CH_2$	$CH_2CH(CH3)_2$
Heptabarbital	C_2H_5	C_7H_{11}
Phenobarbital	C_2H_5	C_6H_5
Secobarbital	$CH_2CH=CH_2$	$CH_3(CH_2)_2CH(CH_3)$
Talbutal	$CH_2CH=CH_2$	$CH(CH_3)CH_2CH_3$

Figure 2.1(b). Barbiturates

Group Environment

The molecular environment of each constituent fragment plays an important role in determining its contribution to the total enthalpy of melting of a compound. The following eight descriptors are used to describe the different molecular environment:

X - A group attached only to sp^3 hybrid atoms

Y - A group attached to one, and only one, sp^2 hybrid atom

YY – A group attached to two sp^2 hybrid atoms

ar - atoms and groups in an aromatic ring

br –atom joining two aromatic rings

bp – biphenyl carbon

ring –atom and groups in an aliphatic ring

fus – atom joining two aliphatic rings

A pictorial representation of these molecular environments is shown in figure 2.2.

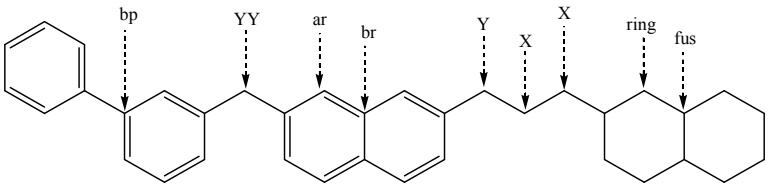


Figure2.2. Molecular environment descriptors in the fragmentation scheme

Proximity factors

In addition to the various molecular fragments, proximity factors for intramolecular hydrogen bonding, geminal halogen atoms and–NH_2 and –OH groups on secondary and tertiary carbons are included in the enthalpy calculation.

Some ortho disubstituted aromatic compounds, as well as some disubstituted trans compounds, can form intramolecular hydrogen bonds. An intramolecular hydrogen bond would reduce the interaction of a molecule with its neighboring molecules, resulting in a

reduced enthalpy of melting and melting point. The proximity factors IHB5, IHB6 and IHB7 are included in our model to account for five, six or seven member intramolecular hydrogen bonded ring formation as shown in figure 2.3. Also shown in the figure is the possibility of a four member intramolecular hydrogen bonded ring. But such ring formation is highly unlikely and there are greater chances of reinforced intermolecular hydrogen bonding resulting in dimerization (Simmamora et al., 1994). Therefore, IHB4 was not considered in our study. In fact, the reinforced hydrogen bonding effect is incorporated in the group contribution values of -COOH and -CONH groups. While assigning the number of possible IHB rings, compounds with two hydrogen donors are given a value of 2 as compared to a count of 1 for compounds with one hydrogen donor. For example, in o-dihydroxybenzene there is a probability for formation of 2 IHB5 rings as compared to a single IHB5 ring in o-chlorophenol.

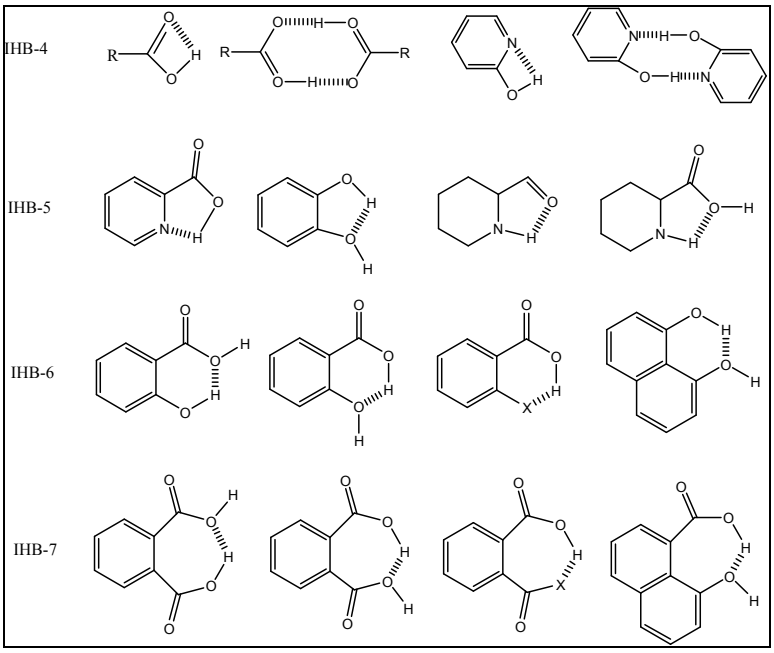


Figure2.3. Intramolecular hydrogen bonding patterns

Three proximity factors are included in the model to account for geminal halogen atoms. A single sp^3 carbon atom containing two, three or four halogen atoms tends to have a reduced enthalpy contribution. This is probably due to the repulsion between the halogen atoms. G2, G3 and G4 are the proximity factors representing a sp^3 carbon containing two, three or four halogen atoms, respectively. Similar proximity factors are included for the steric effects that are associated with –OH and $–NH_2$ groups on secondary and tertiary carbons.

METHODS

Group contribution values were generated using the enthalpy values obtained from the product of experimental melting points and entropies of melting. Contribution values for both the molecular fragments and proximity factors (m_i and m_j) were obtained by multiple linear regressions using SPSS Version 12.0 (SPSS Inc., Chicago, IL).

RESULTS AND DISCUSSION

Multiple linear regression for the enthalpic contribution values of 2230 compounds gives an R-squared value of 0.993 and a standard error of 2.91 kJ/mol. 209 enthalpic contribution values are obtained for the groups, their molecular environment and the proximity factors. Table 2.1 gives a list of all the molecular fragments and proximity factors along with their group contribution values. Each row represents a group and each column represents the group environment.

Table 2.1. A list of molecular fragments and proximity factors along with their enthalpy contribution values

Groups	All	YY	Y	X	ar	br	bp	ring	fus
$-CH_3$	-----	-----	3.24	1.76	-----	-----	-----	-----	-----
$-CH_2$	-----	2.09	2.10	2.95	-----	-----	-----	2.33	-----
$=CH_2$	-----	-----	1.30	-----	-----	-----	-----	-----	-----
>CH-	-----	-0.30	0.67	-0.47	1.59	-----	-----	-0.08	-1.80
=CH-	-----	-----	2.67	-0.67	-----	-----	-----	1.54	-----
≡CH	-----	-----	4.44	-----	-----	-----	-----	-----	-----
>C<	-----	-3.02	0.43	1.19	-0.86	0.18	-0.58	-1.93	-2.28
=C<	-----	-3.68	-----	-1.60	-----	-----	-----	-0.21	-2.28
=C=	-----	0.46	-----	-----	-----	-----	-----	-----	-----
-C≡	-----	-----	0.65	-1.59	-----	-----	-----	-----	-----
-F	-----	-----	2.47	2.03	-----	-----	-----	-----	-----
-Cl	-----	-----	3.48	3.85	-----	-----	-----	-----	-----
-Br	-----	-----	4.47	4.67	-----	-----	-----	-----	-----
-I	-----	-----	5.43	6.58	-----	-----	-----	-----	-----
>N-	-----	-8.66	1.67	1.25	2.39	1.90	-----	0.34	-----
-O-	-----	1.67	4.55	1.57	1.68	-----	-----	4.32	-----
-S-	-----	1.08	4.09	2.81	3.19	-----	-----	6.79	-----
-CN	-----	-----	6.58	6.09	-----	-----	-----	-----	-----
>C(=O)	-----	0.38	3.38	2.35	4.93	-----	-----	4.28	-----
>NH	-----	6.90	6.14	4.71	8.28	-----	-----	3.38	-----
-N=N-	-----	1.63	-----	-----	2.82	-----	-----	-----	-----
-NO-	-----	-----	-----	-----	3.29	-----	-----	-----	-----
-NS-	-----	-----	-----	-----	5.64	-----	-----	-----	-----
-OH	-----	-----	6.16	5.21	-----	-----	-----	-----	-----
-SH	-----	-----	4.34	1.85	-----	-----	-----	-----	-----
>S(=O)	6.42	-----	-----	-----	-----	-----	-----	-----	-----
-P(=O)<	-3.59	-----	-----	-----	-----	-----	-----	-----	-----
-SS-	4.80	-----	-----	-----	-----	-----	-----	-----	-----
$-N_2S-$	-----	-----	-----	-----	8.04	-----	-----	-----	-----
$-NH_2$	-----	-----	5.96	4.14	-----	-----	-----	-----	-----
$-NO_2$	-----	-----	5.89	4.86	-----	-----	-----	9.34	-----
$-SO_2-$	-----	-----	4.21	8.06	-----	-----	-----	-2.84	-----
$-SO_3-$	4.15	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)O-	-----	-----	6.05	4.04	7.95	-----	-----	7.15	-----

Table 2.1. Cont..

Groups	All	YY	Y	X	ar	br	bp	ring	fus
-CH=N	-2.13	-----	-----	-----	-----	-----	-----	-----	-----
-CH=O	-----	-----	5.88	5.54	-----	-----	-----	-----	-----
-C(=O)N<	-----	-----	0.19	3.51	-----	-----	-----	8.80	-----
-SS(=O)-	12.90	-----	-----	-----	-----	-----	-----	-----	-----
-N(=O)=N-	4.72	-----	-----	-----	-----	-----	-----	-----	-----
>NNH-	7.33	-----	-----	-----	11.95	-----	-----	-----	-----
$>NNH_2$	7.28	-----	-----	-----	-----	-----	-----	-----	-----
>NN=O	7.17	-----	-----	-----	-----	-----	-----	-----	-----
$>NNO_2$	8.11	-----	-----	-----	-----	-----	-----	-----	-----
-OC≡N-	7.95	-----	-----	-----	-----	-----	-----	-----	-----
$-ONO_2$	7.44	-----	-----	-----	-----	-----	-----	-----	-----
N≡CC≡N	10.86	-----	-----	-----	-----	-----	-----	-----	-----
>NCH=O	7.91	-----	-----	-----	-----	-----	-----	-----	-----
-OCH=O	4.21	-----	-----	-----	-----	-----	-----	-----	-----
-NH2C≡N	9.80	-----	-----	-----	-----	-----	-----	-----	-----
-NHNH-	11.93	-----	-----	-----	-----	-----	-----	-----	-----
$-NHNH_2$	8.96	-----	-----	-----	-----	-----	-----	-----	-----
$-NHNO_2$	11.91	-----	-----	-----	-----	-----	-----	-----	-----
-NN(R)C(=O)-	-----	-----	-----	-----	13.06	-----	-----	-----	-----
-NNN(R)C(=O)-	-----	-----	-----	-----	4.61	-----	-----	-----	-----
-NN(R)NN-	-----	-----	-----	-----	8.03	-----	-----	-----	-----
-NNNNH-	-----	-----	-----	-----	16.82	-----	-----	-----	-----
>C=NOH	6.06	-----	-----	-----	-----	-----	-----	-----	-----
-CH=NO-	-----	-----	-----	-----	-----	-----	-----	6.78	-----
-CH=NOH	9.65	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)OH	-----	-----	12.15	9.91	-----	-----	-----	-----	-----
-C(=O)Cl	5.45	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)C(=O)-	6.85	-----	-----	-----	-----	-----	-----	-----	-----
-CH=N-N=CH-	6.75	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)NH-	-----	-----	10.59	11.14	9.63	-----	-----	14.05	-----
$-C(=O)NH_2$	-----	-----	12.90	12.92	-----	-----	-----	-----	-----
$-C(=S)NH_2$	16.04	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)NH-	17.57	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=S)NH-	20.23	-----	-----	-----	-----	-----	-----	-----	-----

Table 2.1. Cont..

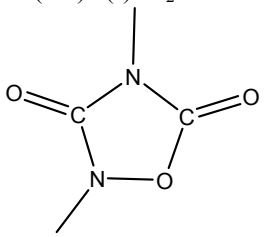
Groups	All	YY	Y	X	ar	br	bp	ring	fus
-$NHCONH_2$	17.57	-----	-----	-----	-----	-----	-----	-----	-----
$NH_2C(=O)NH_2$	18.06	-----	-----	-----	-----	-----	-----	-----	-----
$NH_2C(=S)NH_2$	21.61	-----	-----	-----	-----	-----	-----	-----	-----
>NC(=O)N<	5.81	-----	-----	-----	-----	-----	-----	4.37	-----
>NC(=O)NH-	13.52	-----	-----	-----	-----	-----	-----	-----	-----
$>NC(=O)NH_2$	16.92	-----	-----	-----	-----	-----	-----	-----	-----
-OC(=O)N<	7.58	-----	-----	-----	-----	-----	-----	-----	-----
-OC(=O)NH-	12.48	-----	-----	-----	-----	-----	-----	23.87	-----
$-OC(=O)NH_2$	15.42	-----	-----	-----	-----	-----	-----	-----	-----
-SC(=O)N<	6.82	-----	-----	-----	-----	-----	-----	-----	-----
-SC(=O)S-	-----	-----	-----	-----	9.53	-----	-----	-----	-----
$-SO_2N<$	6.05	-----	-----	-----	-----	-----	-----	-----	-----
$-SO_2NH-$	9.06	-----	-----	-----	-----	-----	-----	-----	-----
$-SO_2NH_2$	4.66	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)NHN<	16.68	-----	-----	-----	-----	-----	-----	-----	-----
$-C(=O)N(NH_2)-$	-----	-----	-----	-----	9.16	-----	-----	-----	-----
-OC(=O)O-	-----	-----	-----	-----	-----	-----	-----	11.78	-----
-ONHC(=O)-	12.53	-----	-----	-----	-----	-----	-----	-----	-----
-OC(=O)C(=O)O-	13.91	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)OC(=O)-	1.07	-----	-----	-----	-----	-----	-----	9.92	-----
-C(=O)N(R)C(=O)-	5.90	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)NHC(=O)-	10.46	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)N(S(R))C(=O)-	9.67	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)NHC(=O)NHC(=O)-	23.10	-----	-----	-----	-----	-----	-----	-----	-----
-C(=O)N(-)SO_2NH-	12.39	-----	-----	-----	-----	-----	-----	-----	-----
	10.36	-----	-----	-----	-----	-----	-----	-----	-----

Table 2.1. Cont..

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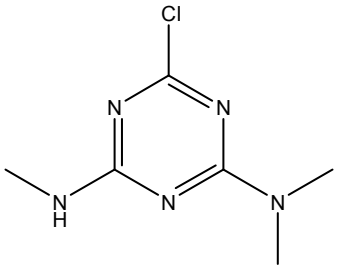
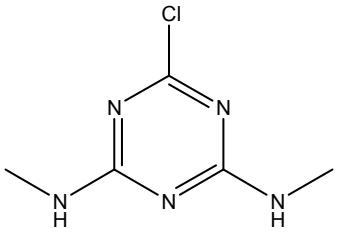
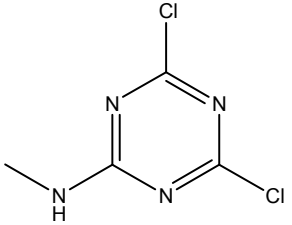
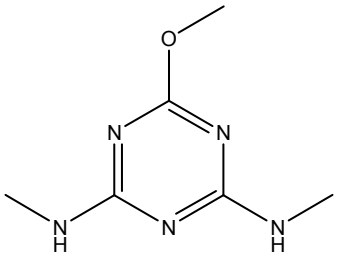
	15.87	-----	-----	-----	-----	-----	-----	-----	-----
	22.51	-----	-----	-----	-----	-----	-----	-----	-----
	18.52	-----	-----	-----	-----	-----	-----	-----	-----
	18.17	-----	-----	-----	-----	-----	-----	-----	-----

Table 2.1. Cont..

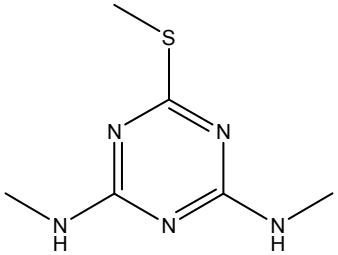
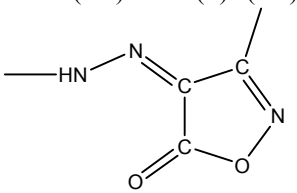
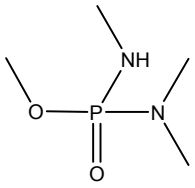
Groups	All	YY	Y	X	ar	br	bp	ring	fus
	19.24	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)CH=NOH	21.70	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)N(R)O-	13.67	-----	-----	-----	-----	-----	-----	-----	-----
>NC(=O)N(R)C(=O)-	9.87	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)NRC(=O)-	11.98	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)NHC(=O)-	17.42	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)ON=C<	12.59	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)ON=CH-	19.15	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)ON=C(-)S-	19.93	-----	-----	-----	-----	-----	-----	-----	-----
-NHC(=O)ON=C(S)C(=O)N<	25.39	-----	-----	-----	-----	-----	-----	-----	-----
	15.54	-----	-----	-----	-----	-----	-----	-----	-----
	5.12	-----	-----	-----	-----	-----	-----	-----	-----

Table 2.1. Cont..

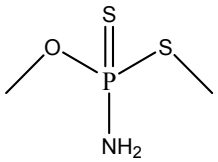
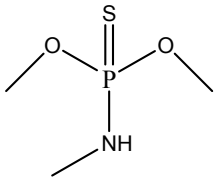
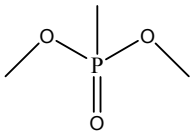
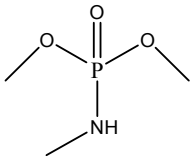
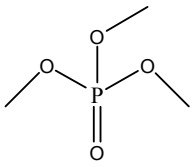
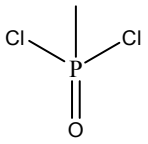
Groups	All	YY	Y	X	ar	br	bp	ring	fus
	14.66	-----	-----	-----	-----	-----	-----	-----	-----
	10.43	-----	-----	-----	-----	-----	-----	-----	-----
	7.41	-----	-----	-----	-----	-----	-----	-----	-----
	7.83	-----	-----	-----	-----	-----	-----	-----	-----
	4.65	-----	-----	-----	-----	-----	-----	-----	-----
	10.30	-----	-----	-----	-----	-----	-----	-----	-----

Table 2.1. Cont..

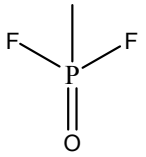
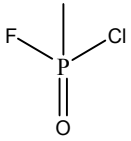
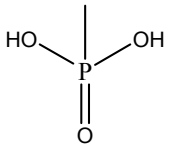
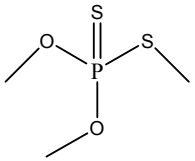
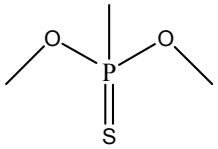
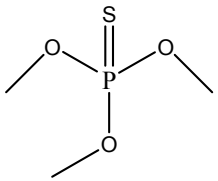
Groups	All	YY	Y	X	ar	br	bp	ring	fus
	7.22	-----	-----	-----	-----	-----	-----	-----	-----
	9.29	-----	-----	-----	-----	-----	-----	-----	-----
	11.07	-----	-----	-----	-----	-----	-----	-----	-----
	6.95	-----	-----	-----	-----	-----	-----	-----	-----
	2.29	-----	-----	-----	-----	-----	-----	-----	-----
	6.50	-----	-----	-----	-----	-----	-----	-----	-----
-SC(=O)N(R)N-	-----	-----	-----	-----	8.21	-----	-----	-----	-----
-SO_2NHC(R)=N-	10.93	-----	-----	-----	-----	-----	-----	-----	-----

Table 2.1. Cont..

Groups	All	YY	Y	X	ar	br	bp	ring	fus
-SO_2NHCH=N-	20.58	-----	-----	-----	-----	-----	-----	-----	-----
-SO_2NHC(=O)-	12.97	-----	-----	-----	-----	-----	-----	-----	-----
-SO_2NHC(=O)NH-	14.71	-----	-----	-----	-----	-----	-----	-----	-----
-SO_2NHC(=O)NHN<	21.56	-----	-----	-----	-----	-----	-----	-----	-----
Proximity factors									
IHB5	-0.19	-----	-----	-----	-----	-----	-----	-----	-----
IHB6	-1.30	-----	-----	-----	-----	-----	-----	-----	-----
IHB7	-0.64	-----	-----	-----	-----	-----	-----	-----	-----
G2	-1.02	-----	-----	-----	-----	-----	-----	-----	-----
G3	-4.64	-----	-----	-----	-----	-----	-----	-----	-----
G4	-7.50	-----	-----	-----	-----	-----	-----	-----	-----
2° OH	5.16	-----	-----	-----	-----	-----	-----	-----	-----
3° OH	4.25	-----	-----	-----	-----	-----	-----	-----	-----
2° NH_2	7.16	-----	-----	-----	-----	-----	-----	-----	-----
3° NH_2	3.54	-----	-----	-----	-----	-----	-----	-----	-----

Note: In the table, R represents an alkyl linkage

The average absolute error in predicting the enthalpy of melting for 1663 compounds using equation (2.1) is 5.5 kJ/mol. It is to be noted that the group contribution values were generated from the entire database of 2230 compounds. However, the errors are calculated for the 1663 compounds with reported enthalpy values. For the remaining compounds with no experimental enthalpy and entropy data, the enthalpy values were generated from the product of experimental melting points and our calculated entropy values. These values were used solely for generating group contributions by multiple regression.

The error distribution obtained while correlating the experimental and predicted enthalpy values which range from 2.3 kJ/mol to 698.9 kJ/mol is shown in figure 2.4.

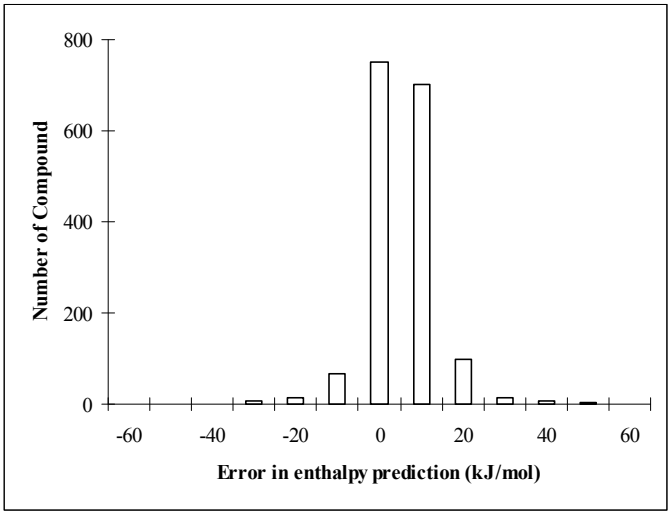


Figure2.4. The distribution of errors in predicting enthalpy of melting

The error distribution in figure 2.4 is fairly symmetrical with a very few outliers. A frequency distribution of the average absolute errors in the prediction of enthalpy of melting is shown in Table 2.2. More than 87% of the compounds have average absolute errors less than 10.0 kJ/mol.

Table 2.2. Frequency distribution of the average absolute errors in enthalpy of melting prediction

Average absolute Error (kJ/mol)	Number of compounds	Cumulative % total
Below 10	1449	87
10-20	168	97
Above 20	46	100

Two examples for predicting enthalpies of melting using the proposed model are shown in Appendix A. A complete list of experimental and calculated enthalpies of melting for the 1663 compounds is given in Appendix B. All compounds are listed in alphanumeric order.

SUMMARY

A group contribution model for calculating enthalpy of melting is developed. The group contributions are generated from a large, complex dataset of over twenty-two hundred organic compounds. The model predicts the enthalpy of melting for 1663 organic compounds which range from 2.3 kJ/mol to 698.9 kJ/mol with an average absolute error of 5.5 kJ/mol. The calculation is simple as it requires only the SMILES notation of a compound as the input parameter. The inclusion of different molecular environment and proximity factors contribute to the accuracy of this model. This model is based on the

isolating carbon rule that distinguishes the large complex molecular fragments that are usually present in drugs and environmental chemicals.

CHAPTER 3: ENTROPY OF MELTING

INTRODUCTION

Total entropy of melting (ΔS_m^{tot}) includes contributions from all solid-solid transitions and the solid-liquid transition. Unlike the enthalpy of melting, it is better understood in geometric terms. By definition, the entropy change associated with melting is related to the relative probabilities of existence of a group of molecules conforming to the geometric restrictions of the liquid and the solid state. Applying the Boltzman relationship to melting, it can be defined as

$$\Delta S_m^{tot} = -R \ln (\Omega^S/\Omega^L) \qquad (3.1)$$

Where Ω^S is the number of ways that 1 mole of a substance can be arranged within the geometric requirements of a crystal and Ω^L is the same for a liquid. According to Bondi (1968), a crystal lattice can place translational, rotational and conformational constraints on its molecules. All of these factors should be included in the estimation of the relative probability of melting. Therefore, the total entropy of melting of a compound is given by:

$$\Delta S_m^{tot} = \Delta S_m^{pos} + \Delta S_m^{rot} + \Delta S_m^{conf} \qquad (3.2)$$

The total entropy of melting mainly consists of the rotational and conformational components; the positional entropy change being relatively small and constant at 15.0 J/K.mol because of the consistent 10-15% increase in volume with melting for organic compounds.

A number of approaches have been used in the past for estimating the total entropy of melting of organic compounds. According to Walden's rule, the entropy of melting for rigid, aromatic compounds is constant with a value of 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 (Jain et al. 2004). Similar to the enthalpy of melting, group contributions have been used in the past for the estimation of entropy of melting (Kirshenbaum, 1965, Chickos et al. 1989, 1999). In their work, Chickos et al. developed a group contribution method for estimating the total entropy of melting with 144 groups. They obtained an average absolute error of 9.9 J/K.mol in predicting the entropy of melting for 1858 organic compounds. While their method has wide applicability, it is cumbersome as it employs a large number of group contribution values and values may be missing for some group fragments.

Although group contributions seem to provide sufficient accuracy in estimation of entropy of melting, entropy is better understood in terms of molecular shape and geometry. In 1979, Martin et al. and Yalkowsky introduced the effects of symmetry and flexibility on the total entropy of melting, respectively. Later, Dannenfelser et al. (1996, 1999) developed a semi-empirical equation combining the effects of rotational symmetry

and molecular flexibility on the total entropy of melting. Their equation is based on only two non-additive molecular parameters,

$$\Delta S_m^{tot} = 50 - 19.1 \log \sigma + 19.1 \log \varphi \qquad (3.3)$$

The rotational entropy is related to the rotational symmetry number (σ); whereas, the conformational entropy is related to the molecular flexibility number (φ) of a compound. These are properties of the whole molecule and are not equal to the sum of the properties of the molecular fragments. They account for the changes in geometrical restriction that accompany the process of melting. In this model, the above equation is used to calculate the total entropy change upon melting.

DATA

The experimental entropies of melting used in this study are the same as described in Chapter 2.

METHODS

Molecular Rotational Symmetry Number

The rotational symmetry number accounts for the likelihood of a molecule being properly oriented for incorporation into the crystal lattice. It is defined as the number of positions into which a molecule can be rotated that are identical to a reference position (Dannenfelser et al., 1996). The rotational symmetry number is an important parameter

for predicting melting points of isomers, e.g. the more symmetric anthracene melts nearly 120° higher than its less symmetrical isomer phenanthrene. By assigning different rotational symmetry numbers for isomers such as phenanthrene (σ=2) and anthracene (σ=4), the model accounts for this large difference in melting points.

While assigning a value to σ, groups such as methyl, hydroxyl, mercapto and primary amines are assumed to be freely rotating and are treated as being radially symmetrical. The nitro and carboxyl groups are treated as laterally symmetrical. All other groups are assumed to be asymmetrical. The rotational symmetry number for a molecule is never less than unity because every molecule has at least one identical orientation that is produced by a 360º rotation about any axis.

Conical (e.g., hydrogen cyanide and chloromethane) and cylindrical (e.g., carbon dioxide and ethane) molecules are empirically assigned symmetry numbers of 10 and 20, respectively. Spherical molecules (e.g., neon and methane) are assigned a symmetry number of 100. All flexible molecules are assigned a symmetry number of unity. Examples of rotational symmetry for a number of molecules are shown in figure 3.1.

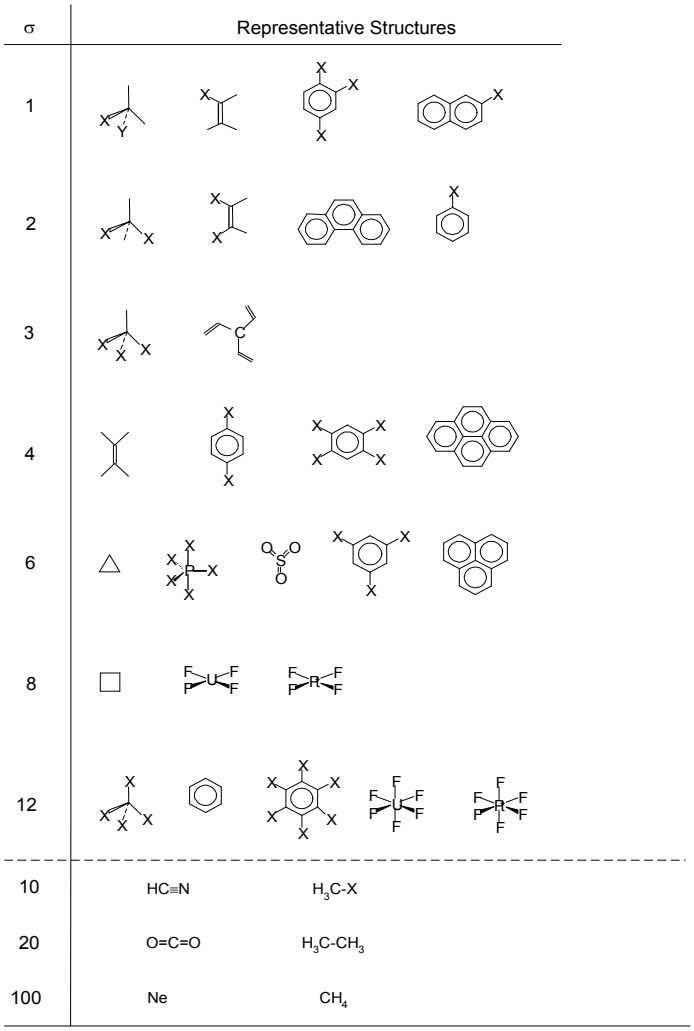


Figure 3.1. Symmetry numbers for several molecules

Molecular Flexibility Number

The molecular flexibility number (φ) is an exponential function of chain length and is calculated by:

$$\varphi = 2.435^{\Phi} \qquad (3.4)$$

So that

$$19.1 \log \varphi = 7.4\Phi \qquad (3.5)$$

Φ denotes the number of torsional angles or the flexibility count of a molecule. The flexibility count for any compound can be calculated using the following semi-empirical equation of Dannenfelser et al. (1999):

$$\Phi = SP3 + 0.5SP2 + 0.5RING - 1 \qquad (3.6)$$

Where SP3 = Σ Nonring (CH_2, CH, C, NH, N, O, S)
SP2 = Σ Nonring (=CH, = C, = N, C=O)
Ring = Σ Independent single, fused, or conjugated ring systems

The value 2.435 in equation 3.4 is based upon theoretical calculations by Tonelli (1970), Kirshenbaum (1965) and Starkweather et al. (1960) which state that the conformational entropy of melting for an isolated polyethylene chain is 7.4 ± 0.2 J/K.mol per four-atom torsional unit. These calculations are based on the assumptions that the trans conformation is more stable than the gauche conformations and the gauche (+) - gauche (-) sequences are hindered or forbidden.

In the flexibility count, terminal groups such as CH_3, NH_2, OH, CN, F, Cl, Br, I, =O, $=CH_2$, and ≡N as well as non-terminal sp hybrid carbons are not included. Also not included are carbon atoms with three identical groups, for example, trihalomethyl or tert-

butyl groups. Compounds with a negative value for Φ are assigned a value of 0. For compounds containing aliphatic cyclic rings such as cyclohexane, a value of -2 per ring is added (Jain et al., 2004). A few examples of molecular flexibility numbers are shown in Table 3.1.

Table 3.1. Examples of some molecular flexibility numbers

Name	σ	SP3	SP2	RING	Φ	φ
n-pentane	1	3	0	0	2	5.93
2-methylbutane	1	2	0	0	1	2.44
neopentane	1	1	0	0	0	1.00
1-pentanol	1	4	0	0	3	14.44
3-pentanone	1	2	1	0	1.5	3.80
cyclopentane	0	5	0	0	2	5.93
toluene	2	0	0	1	0	1.00
tert-butylbenzene	2	0	0	1	0	1.00
1,2,4 trimethylbenzene	1	0	0	1	0	1.00
1,3,5-trimethylbenzene	6	0	0	1	0	1.00
4-chlorophenol	2	0	0	1	0	1.00
benzoic acid	2	0	0	1	0	1.00
2,4,6-trinitrotoluene	2	0	0	1	0	1.00
n-butylbenzene	1	3	0	1	2.5	9.25
hexamethylbenzene	12	0	0	1	0	1.00

RESULTS AND DISCUSSION

The average absolute error in predicting the total entropy of melting for 1663 compounds using equation (3.3) is 15.0 J/K.mol. The error distribution obtained while correlating the experimental and predicted entropy values which range from 8.5 J/K.mol to 1751.2 J/K.mol is shown in figure 3.2.

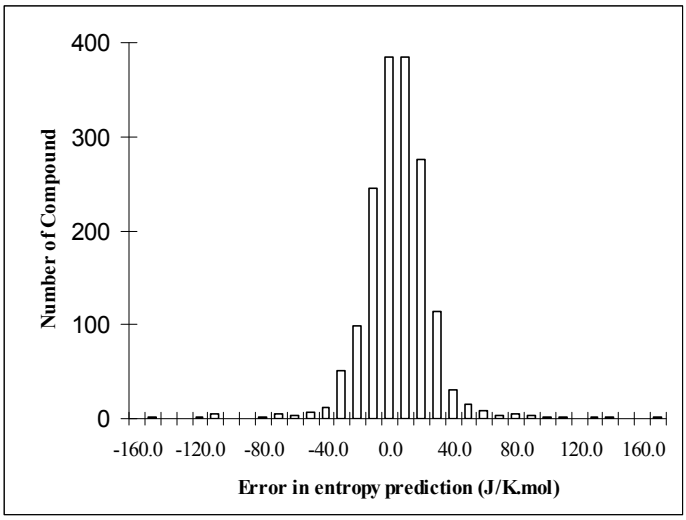


Figure3. 2. The distribution of errors in predicting entropy of melting

As seen in Figure 3.2, the error distribution is fairly symmetrical with a very few outliers. A majority of the outliers are the very long chain flexible molecules similar to those seen in enthalpy calculations. Figures 3.3 and 3.4 show the distribution of errors as a function of the logarithm of the rotational symmetry number (σ) and molecular flexibility count (Φ). In Figure 3.3, an almost symmetric distribution of errors is observed at each rotational symmetry number. On the other hand, as seen in Figure 3.4, at low flexibility counts the errors are distributed symmetrically but as the flexibility count increases, the distribution becomes more random with a large proportion of outliers. Such long chain, flexible molecules are very likely to form liquid crystals and exhibit mesophasic behavior and multiple transitions before the actual melting to the isotropic liquid. Sometimes the entropies associated with all these transitions are not accounted for in the reported

experimental entropy values. This leads to an increase in the average error associated with their entropy predictions.

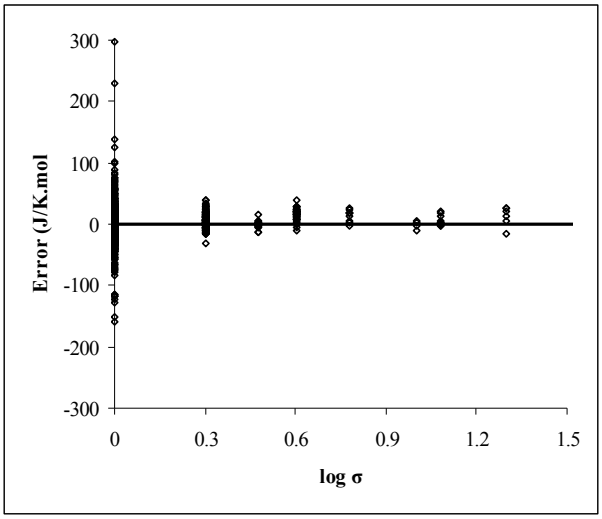


Figure 3.3. Error distribution as a function of the logarithm of the rotational symmetry number (σ)

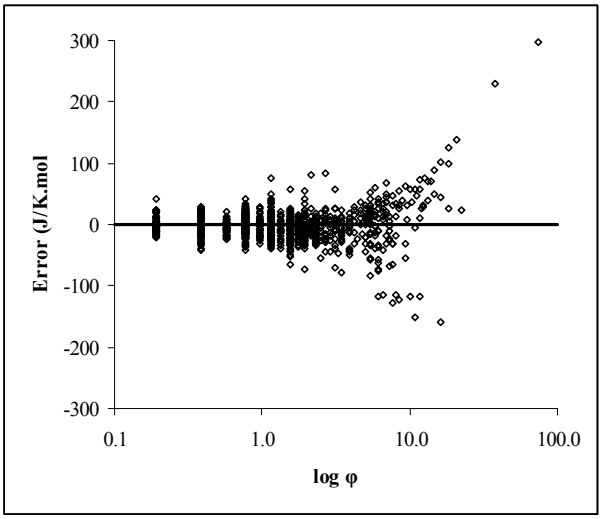


Figure3. 4. Error distribution as a function of the logarithm of the molecular flexibility number (φ). Note that the x-axis is on a logarithmic scale.

The effect of the large errors in entropy prediction for very long chain flexible molecules on the overall absolute average error can be seen in Table 3.2. The average absolute error increases as longer chain compounds are included in the dataset. It is evident that equation 3.3 gives better estimations of entropy of melting for compounds with lower flexibility counts.

Table 3.2. Average absolute errors in entropy of melting prediction at different flexibility count (Φ)

Flexibility count (Φ)	Number of compounds	Average absolute Error (J/K.mol)
Below 5	1380	11.8
5-10	123	18.4
10-15	72	21.0
Above 15	88	54.5

Table 3.3 gives a frequency distribution of the average absolute errors in the prediction of total entropy of melting for 1663 compounds. More than 77% of the compounds have average errors less than 20 J/K.mol.

Table 3.3. Frequency distribution of the average absolute errors in entropy of melting prediction

Average absolute Error (J/K.mol)	Number of compounds	Cumulative %total
Below 20	1286	77
20-40	297	95
40-60	43	98
Above 60	37	100

Two examples for predicting entropies of melting using the proposed model are shown in Appendix A. A complete list of experimental and calculated entropies of melting for the 1663 compounds is given in Appendix C. Also listed are the rotational symmetry number (σ) and flexibility count (Φ) for each compound. All compounds are listed in alphanumeric order.

SUMMARY

The semi-empirical equation of Dannenfelser and Yalkowsky (equation 3.3) is validated on a large database of pharmaceutically and environmentally relevant organic compounds. This equation predicts the total entropies of melting for over 1600 organic compounds with an average absolute error of 15.0 J/K.mol. It is a reasonable estimate considering that no coefficients were generated from experimental data for a training set.

CHAPTER 4: MELTING POINTS

INTRODUCTION

Melting Point is one of the most widely reported physical properties for organic compounds. Despite the availability of vast amounts of experimental melting point data, there is no general relationship relating melting point directly to chemical structure. A simple method that can estimate melting points directly from chemical structure would be a valuable tool in pharmaceutical and environmental science. Such a method would assist in the evaluation and design of new drug derivatives and chemicals that would be within a specified range of melting point, solubility, and vapor pressure.

A number of attempts have been made to correlate melting points to chemical structure. Broadly, these methods fall into three categories: additive group contributions, non-group QSPR methods, and the enthalpy/entropy combinations.

Group contribution methods are the simplest of all methods but they are associated with greater errors. One of the primary reasons for these larger errors is their inability to distinguish between isomers. Some of the significant group contribution methods for estimation of melting points were developed by Joback et al. (1987), Constantinou et al. (1994) and Marrero et al. (2001). Joback et al. developed a first-order group contribution method with 40 groups for organic compounds containing halogens, oxygen, nitrogen and sulfur. Constantinou et al. came up with a two-level group contribution scheme consisting of 63 first-order groups and 40 second-order groups. While the first-order

groups accounted for the groups similar to those of Joback et al., the second-order groups helped distinguish between isomers and accounted for some proximity factors. Inclusion of second-order groups provides greater accuracy but at the same time, the method is time consuming and difficult to use. Marrero et al. updated this model further to include third-order groups that could account for more complex heterocyclic and large polyfunctional alicyclic compounds. This method has 165 first-order groups, 115 second-order groups and 64 third-order groups. This method is advantageous in terms of its greater accuracy and wide applicability. However the large number of groups makes it cumbersome.

A number of QSPR methods are available for estimation of melting points. These methods are based on specific families of compounds, and their application is limited to these specific families. Alkanes (Charton et al. 1994, Needham et al. 1988), aldehydes, amines, ketones (Katritzky et al. 1993, Dearden, 1991) and benzenes (Katritzky et al. 1997) are some of the families for which QSPR models have been developed. According to a recent review by Katritzky et al. (2003), the current QSPR methods range in accuracy from very good (standard deviation = 15.1K for n-alkanes) to similar accuracy as group contributions (standard deviation = 36.1K for pyridines). The major disadvantage of QSPR methods is their limited application to the specific class of compounds they are based on.

Melting points can also be estimated from the ratio of the enthalpy and entropy of melting. Enthalpy of melting is estimated by group contributions whereas the entropy of

melting is correlated from QSPR descriptors for symmetry and flexibility. Such correlations have been developed for alkanes (Tsakanikas et al. 1988), aliphatics (Zhao et al. 1999, Krzyzaniak et al. 1995) and aromatic compounds (Simamora et al. 1993).

In addition to the above mentioned methods, Chickos et al. (2001) developed a parabolic model for estimating the melting points of homologous series. In yet another method developed by Yalkowsky et al., the melting points were estimated from the boiling points of organic compounds. The average absolute errors (AAE), number of compounds and compound categories for some of the methods discussed above are listed in Table 4.1.

Table 4.1. Average Absolute Errors in general melting point estimation methods

Method	Number of Compounds	AAE	Compound Class
Tsakanikas et al.	72	15.7	Alkanes
Simamora et al.	123	47.6	Rigid Aromatic
Krzyzaniak et al.	497	30.3	Non H-bonding Aliphatic
Zhao et al.	794	39.9	Aliphatic
Yalkowsky et al.	918	31.7	from Boiling Point
Constantinou et al.	1007	34.6	Organic
Joback et al.	1117	43.0	Organic
Marrero et al.	1170	32.4	Organic

Selection of a melting point estimation method is dependent upon the level of desired accuracy and applicability. QSPR models have greater accuracy in their particular class of compounds but their extrapolation to compounds outside the training set leads to very poor correlations. Group contribution schemes fail to distinguish between isomers and

result in greater errors. The more general enthalpy/entropy combination approaches have wider applicability and are more valuable in cases where compounds do not fit within well-defined families or belong to families for which QSPR methods do not exist.

This chapter describes our melting point estimation model that is based on the combination of enthalpy and entropy using a large dataset of over 2200 organic compounds.

DATA

The experimental data for melting points used in this study is the same as described in Chapter 2.

METHODS

The melting point denotes the temperature at which a crystalline solid is transformed into a liquid. At the melting point, the free energy of transition is equal to zero and the thermodynamic expression for melting point is given by

$$T_m = \frac{\Delta H_m}{\Delta S_m} \qquad (4.1)$$

Where

T_m = Melting point (K)

ΔH_m = total phase change enthalpy of melting (kJ/mol)

ΔS_m = total phase change entropy of melting (J/K.mol)

The enthalpy and entropy of melting are calculated as described in Chapters 2 and 3 respectively.

RESULTS AND DISCUSSION

As described in equation 4.1, the melting points are estimated from the ratio of the enthalpy and entropy of melting. The average absolute error is 30.1° for melting points ranging from 85.5 K to 710.5 K.

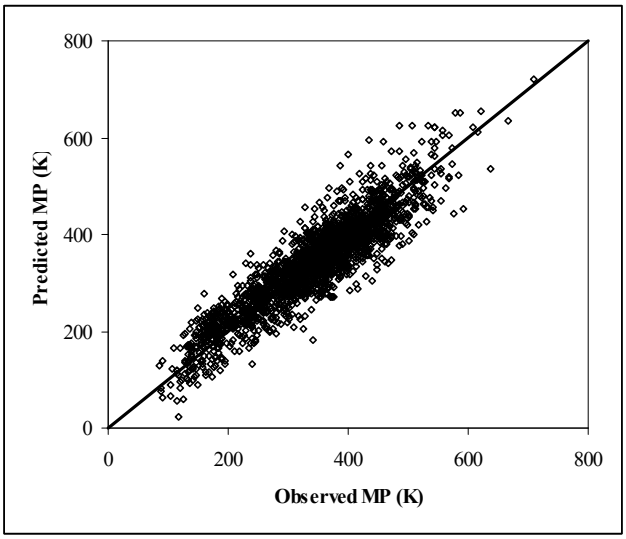


Figure4.1. Observed versus predicted melting points for 2230 organic compounds

Figure 4.1 shows a plot of predicted versus observed melting points for the entire data set. The narrow distribution of values along the line of identity suggests an accurate prediction using the proposed model. Most of the values are overlapping because of the large number of observations in the study.

Figure 4.2 shows the error distribution obtained in correlating the experimental and predicted melting points. The distribution is fairly symmetrical with few outliers.

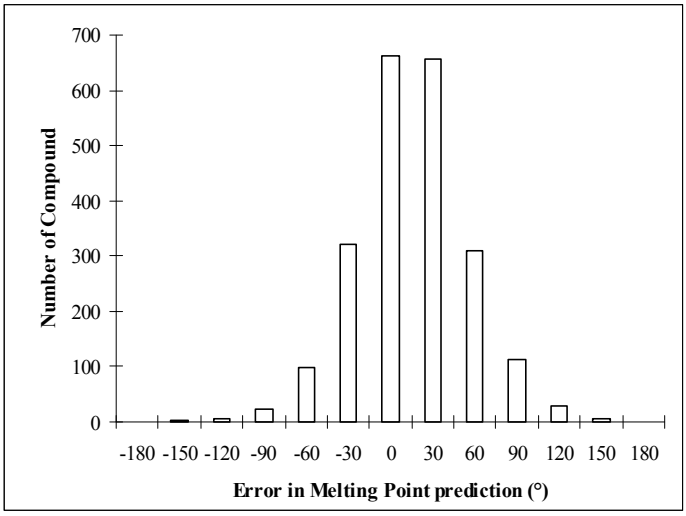


Figure4.2. Error distribution in melting point prediction using the proposed model

Table 4.2 gives a frequency distribution of the average absolute errors in melting point prediction. Only 2% of the compounds have average absolute errors greater than 100°. It is to be noted that a 100° error corresponds to a ten-fold error in calculated solubility by Yalkowsky's General Solubility Equation (Ran et al., 2001).

Table 4.2. Frequency distribution of the average absolute errors in melting point prediction

Average absolute Error	Number of compounds	Cumulative % total
Below 30°	1320	59
30°-60°	630	87
60°-90°	211	97
Above 90°	69	100

A three-fold cross validation was performed on the database to validate the prediction ability of this method. For each validation, approximately $1/10^{th}$ of the data was selected at random (RAND function, Microsoft Excel 2000) and used as the test set. The remaining data were used as the training set to generate the group contribution values. Average absolute errors were calculated for each pair of test and training sets. The results for cross validation are listed in Table 4.3, where N represents the number of compounds in each set. The similarity of the absolute errors for the test and training sets and the overall absolute error strongly validates the predictability of this method.

Table 4.3. Cross-validation of proposed method

Cross Validation	Training Set		Test set	
	AAE	N	AAE	N
Round 1	29.9°	2007	33.1°	222
Round 2	29.7°	2007	37.2°	218
Round 3	30.0°	2007	33.8°	216

AAE = Average absolute error in melting point prediction, N = number of compounds

The accuracy of melting point predictions obtained with the proposed model is attributed mainly to the separate calculation of the enthalpy and entropy of melting. This is a distinct advantage over group contribution methods that are incapable of accounting for the effect of symmetry and flexibility. The chemical diversity of over twenty-two hundred compounds studied illustrates the fact that this model has wide applicability. It gives melting point predictions ranging over nearly nine orders of magnitude with an average absolute error of 30°.

In addition, we are able to predict melting points of complex structures including many drugs, steroids, herbicides and pesticides. The identification and inclusion of large, complex molecular fragments using the isolating carbon concept is a useful tool for calculating the enthalpy of melting and subsequently the melting points of these complex structures.

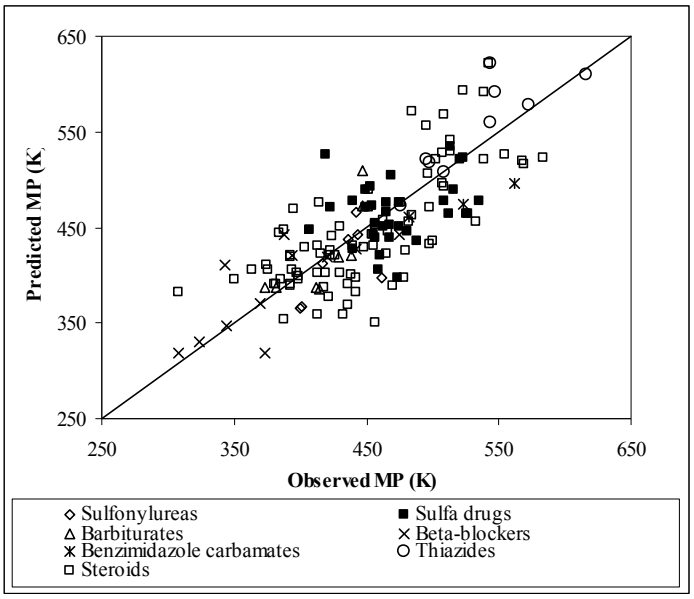


Figure4.3. Predicted versus observed melting points for 152 drugs (including steroids) in the database

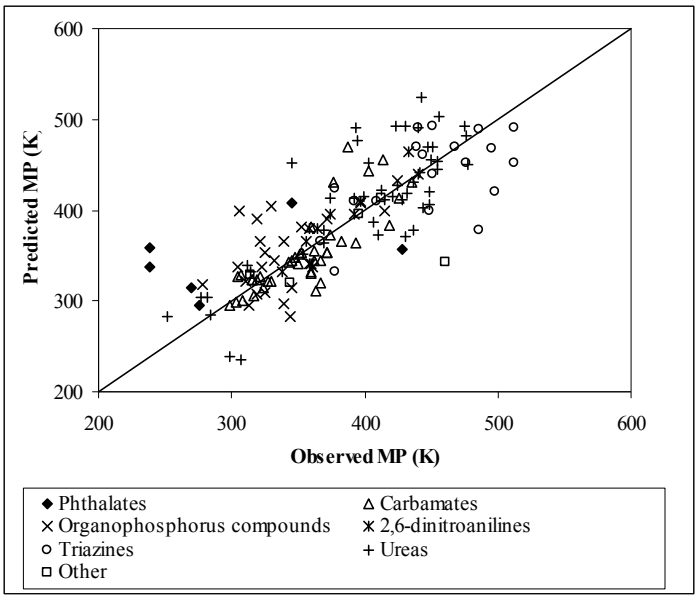
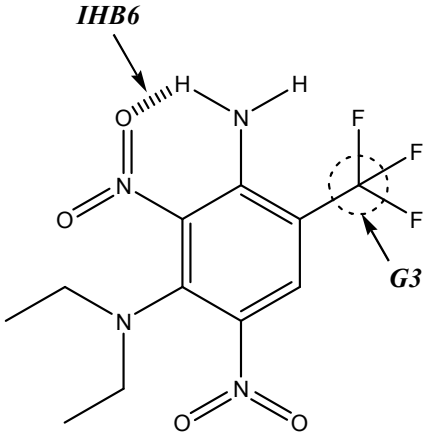


Figure4.4. Predicted versus observed melting points for 149 environmental compounds included in the database

Figure 4.3 and 4.4 show the observed versus predicted melting points of 152 drugs (including steroids) and 149 environmental compounds respectively. In both cases, the distribution of values along the line of identity is narrow. The melting points of about 75% of the drugs and 85% of the environmental compounds are off by less than 50°. The proximity factors for intramolecular hydrogen bonding, geminal halogen atoms and –OH and $–NH_2$ groups on secondary and tertiary carbons contribute to accurate enthalpy of melting and melting point predictions. For example, as seen in Figure 4.5, a large improvement is observed in the melting point prediction of dinitramine when proximity factors for intramolecular hydrogen bond and geminal halogens are included in the enthalpy calculation.



Observed Melting Point: 372.1 K
Predicted Melting Point (no proximity factors): 459.1 K
Predicted Melting Point (with proximity factors): 390.0 K

Figure4.5. Proximity factors for intramolecular hydrogen bonding and geminal fluorine atoms in dinitramine

Two examples for predicting melting points using the proposed model are shown in Appendix A. A complete list of the 2230 organic compounds along with their observed and predicted melting points is provided in Appendix D. The compounds are arranged in alphanumeric order.

The proposed model is in agreement with the principle of convergence temperature. When the proposed model was applied to a dataset of 40 linear alkanes ranging from C2-C190, a convergence similar to the experimental melting points was observed as seen in Figure 4.6.

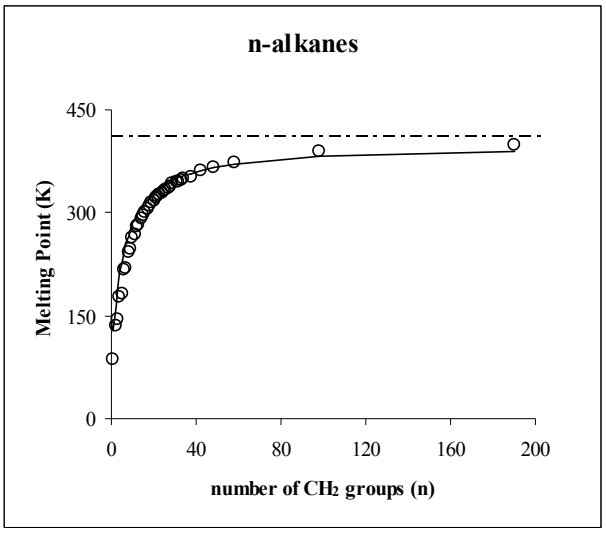


Figure 4.6. Experimental melting points of n-alkanes (C2-C190) (○). The dotted line represents predicted values. The dashed line represents the convergence temperature at 410.0 K.

Addition of a methylene group to a linear hydrocarbon increases its van der Waals interaction energy and thus its enthalpy of melting by a constant value. This would suggest a linear increase in melting-points with an increase in chain length. However, with an increase in the number of methylene groups, the flexibility term becomes an important factor and it adds to the entropy of melting by a constant value. If the enthalpy and entropy of melting are expressed as linear functions of chain length (n), melting point equation can be written as

$$T_m = \frac{\Delta H_m}{\Delta S_m} = \frac{a + bn}{c + dn} \tag{4.2}$$

Similar equations were derived by Broadhurst (1963) and Flory and Vrij (1963). Chickos and Nichols (2001) developed a hyperbolic function of chain-length to estimate the melting temperatures of homologous series. According to the above equation, as $n \rightarrow \infty$, T_m approaches a limiting value of b/d, also known as the convergence temperature. For alkanes, this value has been experimentally determined to be 410 K (dashed line in Figure 4.6). Based on an enthalpic group contribution value of 2.95 kJ/mol and an entropy value of 7.382 $JK^{-1}mol^{-1}$ for a methylene group, the proposed method estimates the convergence temperature for alkanes to be 399.6 K.

SUMMARY

Melting points are predicted for a chemically diverse database of 2230 organic compounds with an average absolute error of 30.1°. The proposed model provides an accurate and widely applicable tool for predicting melting points directly from molecular structure.

CHAPTER 5: COMPARISON OF TWO METHODS FOR PREDICTING MELTING POINTS

INTRODUCTION

In this chapter, the melting point predictions of UPPER as described in this dissertation are compared to those of MPBPWIN for 2230 organic compounds. MPBPWIN is a program available through the Environmental Protection Agency. It predicts melting points using two different group contribution methods.

DATA

The dataset used in this study is the same as used in Chapters 2, 3 and 4.

METHODS

In UPPER, melting points are calculated using the following relationship:

$$T_m = \frac{\Delta H_m}{\Delta S_m} \qquad (5.1)$$

Where

T_m = Melting point (K)

ΔH_m = total phase change enthalpy of melting (kJ/mol)

ΔS_m = total phase change entropy of melting (J/K.mol)

The total phase change enthalpy and entropy of melting were calculated as described in Chapters 2 and 3 respectively.

MPBPWIN estimates melting points using two different group contribution methods. The first method is based on the group contribution scheme developed by Joback (1984) and Reid et al. (1987). The second method was suggested by Lyman (1985) and was originally developed by Gold et al. (1969). In this method, the melting points are calculated from the boiling points using the following relationship:

$$T_m = 0.5839 T_b \tag{5.2}$$

The boiling points (Tb) used in this equation are obtained by group contributions. In addition, the MPBPWIN program also contains correction factors for specific structures.

In order to evaluate the two models, average absolute errors (AAE) and root mean square errors (RMSE) were calculated for each method.

AAE was determined by

$$AAE = \frac{\sum \left| T_{m,obs} - T_{m,pred} \right|}{N} \tag{5.3}$$

N = number of compounds

RMSE was determined by

$$RMSE = \sqrt{\frac{\Sigma(T_{m,obs} - T_{m,pred})^2}{N}} \quad (5.4)$$

N = number of compounds

RESULTS AND DISCUSSION

Plots of observed versus predicted melting points for the 2230 organic compounds by each method are shown in Figures 5.1 and 5.2. As seen in the two figures, UPPER based melting point estimation model has an R-squared value of 0.830 whereas MPBPWIN has an R-squared value of 0.645.

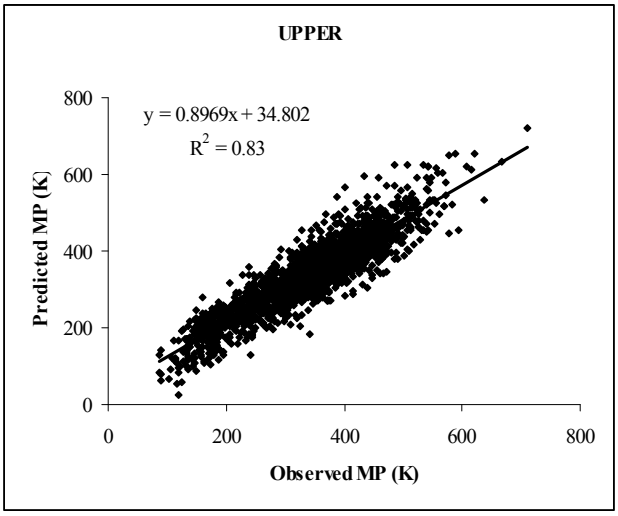


Figure 5.1. Observed versus predicted melting points (using UPPER) for 2230 compounds

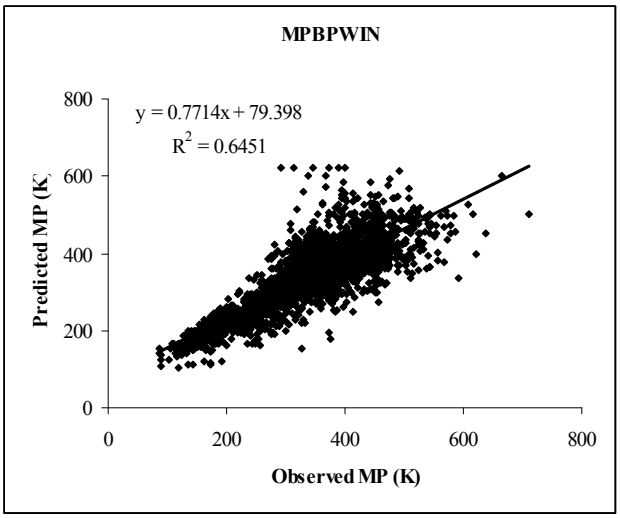


Figure 5.2. Observed versus predicted melting points (using MPBPWIN) for 2230 compounds

The AAE for UPPER is 30.1° as compared to 44.5° for MPBPWIN. Also the RMSE for UPPER (39.7°) is considerably lower than that obtained using MPBPWIN (58.4°). These values clearly indicate that the UPPER model provides a better prediction of melting points as compared to MPBPWIN for a large, diverse set. The greater accuracy of UPPER melting point predictions is based on the fact that it accounts for both the additive and non-additive aspects of the melting process. MPBPWIN, which is based solely on additive group contributions, does not account for the geometric factors involved in melting. Group contribution alone cannot distinguish between the melting points of isomers that have, in instances, melting points differing by over 100°. In contrast, UPPER includes the entropy of melting in its melting point prediction. The entropy of melting term consists of the rotational symmetry number that differentiates between isomers and the flexibility number that accounts for the conformational changes upon melting, especially for long, flexible molecules.

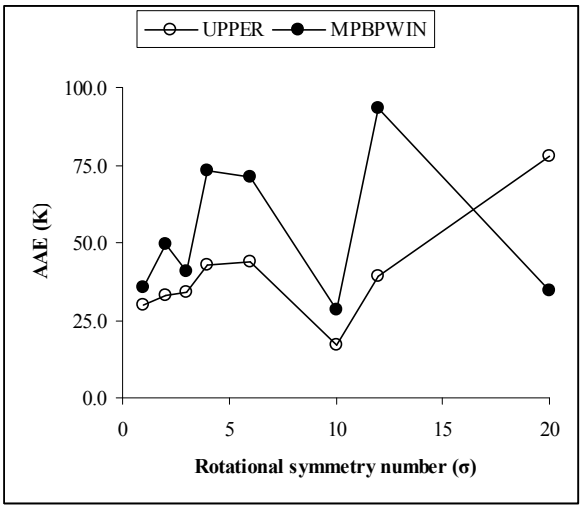


Figure 5.3. AAE in melting point prediction of symmetrical molecules using the two models

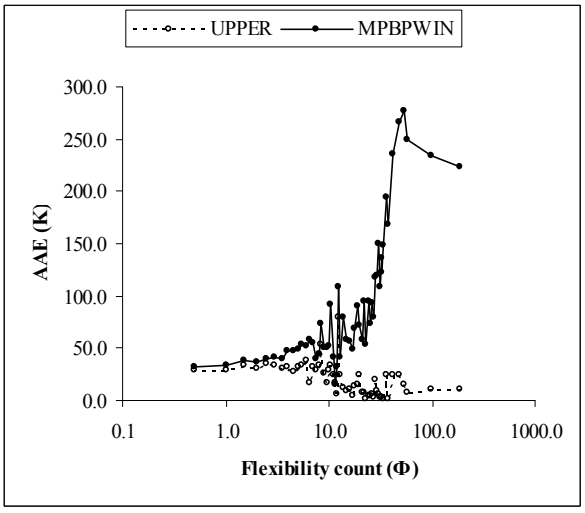


Figure 5.4. AAE in melting point predictions of flexible molecules using the two models. Note that the x-axis is on a logarithmic scale

Figures 5.3 and 5.4 are plots of AAE for each method versus the rotational symmetry number and the flexibility number respectively. To reduce the number of data points, the AAE for compounds having same symmetry number or flexibility number are averaged.

It is evident from both figures that UPPER consistently provides more accurate predictions of melting points for a diverse set of compounds, ranging from highly symmetrical rigid molecules to long, flexible molecules.

In addition, the enthalpy calculation in UPPER is based on a group contribution scheme. This scheme is based on the isolating carbon rule and is of great utility in identifying complex molecular fragments often encountered in chemical structures of drugs and pesticides. The scheme also contains proximity factors like intramolecular hydrogen bonding and geminal halogen atoms. A combination of this additive group contribution scheme and the non-additive entropic contributions results in a melting point estimation model that is reasonably accurate and widely applicable.

SUMMARY

Two widely applicable models for predicting melting points directly from chemical structure are compared. The average absolute error (AAE) and root mean square error (RMSE) in melting point prediction using UPPER are 30.1° and 39.7°, while MPBPWIN gives an AAE of 44.5° and RMSE of 58.4°. UPPER provides more accurate melting point predictions because it accounts for both the additive enthalpic and non-additive entropic contributions to melting.

APPENDIX A. Examples of predicting enthalpy of melting (ΔH_m), entropy of melting (ΔS_m) and melting point (T_m) using the developed model.

(a) Butanoic Acid

CH_3-CH_2-CH_2-C(=O)(OH)

Parameters: Observed T_m = 264.7 K, σ = 1, $\Phi = 2.435^{(1.5)}$

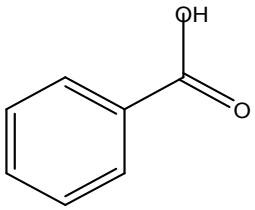
$\Delta H_m = \Sigma n_i m_i$ = 1(XCH3) + 1(XCH2) + 1(YCH2) + 1(XCOOH)

= 1(1.76) + 1(2.95) + 1(2.10) + 1(9.91) = 16.72 kJ/mol

$\Delta S_m = 50 - R \ln \sigma + R \ln \phi = 50 - 8.31 \ln(1) + 8.31 \ln [2.435^{(1.5)}] = 61.1$ J/K.mol

$T_m = \Delta H_m / \Delta S_m$ = 16720 / 61.1 = 273.6 K

(b) Benzoic acid



Parameters: Observed T_m = 395.5 K, σ = 2, $\Phi = 2.435^{(0)}$

$\Delta H_m = \Sigma n_i m_i$ = 1(Car) + 5(CHar) + 1(YCOOH)

$= 1(-0.86) + 5(1.59) + 1(12.15) = 19.24$ kJ/mol

$\Delta S_m = 50 - R \ln \sigma + R \ln \phi = 50 - 8.31 \ln(2) + 8.31 \ln [2.435^{(0)}] = 44.2$ J/K.mol

$T_m = \Delta H_m / \Delta S_m = 19240 / 44.2 = 435.3$ K

APPENDIX B. Experimental and predicted enthalpy of melting (ΔH_m) for 1663 organic compounds.

Name	ΔH_m (kJ/mol)	
	experimental	predicted
(+)2-butanol	6.00	11.16
(+)a-(3-benzoylphenyl)propionic acid	28.23	23.47
(2,4,5-trichlorophenoxy)acetic acid	38.00	26.72
(2,4-dichlorophenoxy)acetic acid	35.33	25.69
(4-chloro-2-methylphenoxy)acetic acid	29.98	25.46
(4-chloro-o-tolyloxy)acetic acid	29.98	25.46
(d) 1,2-dibromoacenaphthene	26.36	19.41
(d) 1,2-dichloroacenaphthene	21.34	17.77
(d) 1,2-diphenyl-1,2-dihydroxyethane	34.31	25.83
(d) 2-(1-naphthoxy)propionamide	38.07	30.52
(D) 2-(2-chloro-3-methylphenoxy)propionic acid	22.18	25.79
(d) 2-(m-chlorophenoxy)propanoic acid	29.71	25.00
(d) 2-(o-chlorophenoxy)propanoic acid	26.78	25.00
(d) 2-(p-bromophenoxy)propanoic acid	27.61	25.99
(d) 2-(p-methoxyphenyl)propiophenone	21.76	22.87
(d) 2-(p-nitrophenoxy)propanoic acid	20.92	27.41
(d) 2,3-dibromo-1,4-butanediol	33.89	24.72
(d) 2-phenoxypropionic acid	22.59	23.97
(d) 3-(m-bromophenyl)-3-hydroxypropanoic acid	23.85	26.94
(d) 3-(m-chlorophenyl)-3-hydroxypropanoic acid	28.03	25.95
(d) 3-(m-fluorophenyl)-3-hydroxypropanoic acid	24.27	24.94
(d) 3-(o-fluorophenyl)-3-hydroxypropanoic acid	22.59	24.94
(d) 3-(p-bromophenyl)-3-hydroxypropanoic acid	35.56	26.94
(d) 3-(p-chlorophenyl)-3-hydroxypropanoic acid	28.03	25.95
(d) 3-(p-fluorophenyl)-3-hydroxypropanoic acid	30.96	24.94
(d) 3-hydroxy-3-phenylbutyric acid	22.59	25.53
(d) 3-hydroxy-3-phenylvaleric acid	30.96	28.48
(d) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid	39.75	26.78
(d) 3-phenyl-3-hydroxypropanoic acid	32.64	24.92
(d) dimethyl diacetyltartrate	29.29	27.49
(d) dimethyl tartrate	17.36	23.06
(d) malic acid	23.01	27.55
(d) mandelic acid	26.36	21.85
(d) methylenebisthiopropionic acid	22.59	33.26
(d) m-fluoromandelic acid	24.27	21.88
(d) o-chloromandelic acid	24.69	22.88
(d) o-fluoromandelic acid	20.92	21.88
(d) p-chloromandelic acid	23.01	22.88
(d) p-fluoromandelic acid	30.54	21.88
(dl) 1,2-dibromoacenaphthene	25.10	19.41
(dl) 1,2-dichloroacenaphthene	20.50	17.77
(dl) 1,2-diphenyl-1,2-dihydroxyethane	31.38	25.83
(dl) 2-(1-naphthoxy)propionamide	37.66	30.52
(dl) 2-(2-chloro-3-methylphenoxy)propionic acid	30.54	25.79
(dl) 2-(m-chlorophenoxy)propanoic acid	33.05	25.00

(dl) 2-(o-chlorophenoxy)propanoic acid	32.22	25.00
(dl) 2-(p-bromophenoxy)propanoic acid	31.80	25.99
(dl) 2-(p-methoxyphenyl)propiophenone	26.36	22.87
(dl) 2-(p-nitrophenoxy)propanoic acid	32.22	27.41
(dl) 2,3-dibromo-1,4-butanediol	29.29	24.72
(dl) 2-phenoxypropionic acid	33.05	23.97
(dl) 3-(m-bromophenyl)-3-hydroxypropanoic acid	26.78	26.94
(dl) 3-(m-chlorophenyl)-3-hydroxypropanoic acid	23.85	25.95
(dl) 3-(m-fluorophenyl)-3-hydroxypropanoic acid	20.50	24.94
(dl) 3-(o-fluorophenyl)-3-hydroxypropanoic acid	27.20	24.94
(dl) 3-(p-bromophenyl)-3-hydroxypropanoic acid	28.87	26.94
(dl) 3-(p-chlorophenyl)-3-hydroxypropanoic acid	29.71	25.95
(dl) 3-(p-fluorophenyl)-3-hydroxypropanoic acid	27.61	24.94
(dl) 3-hydroxy-3-phenylbutyric acid	19.66	25.53
(dl) 3-hydroxy-3-phenylvaleric acid	35.15	28.48
(DL) 3-methylnonane	18.70	22.51
(dl) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid	37.24	26.78
(dl) 3-phenyl-3-hydroxypropanoic acid	29.71	24.92
(DL) 4-methylnonane	15.19	22.51
(dl) dimethyl diacetyltartrate	25.94	27.49
(dl) dimethyl tartrate	26.94	23.06
(dl) malic acid I	33.52	27.55
(dl) malic acid II	30.17	27.55
(dl) mandelic acid	25.52	21.85
(dl) menthol	10.25	16.71
(dl) methylenebisthiopropionic acid	39.33	33.26
(dl) m-fluoromandelic acid	24.69	21.88
(dl) o-chloromandelic acid	20.08	22.88
(dl) o-fluoromandelic acid	30.12	21.88
(dl) p-chloromandelic acid	27.20	22.88
(dl) p-fluoromandelic acid	29.29	21.88
(l) menthol	11.88	16.71
[(benzoylamino)oxy] acetic acid	31.46	31.62
1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	22.87	28.82
1-(methylamino)-9,10-anthracenedione	28.81	27.42
1-(o-chlorophenyl)thiourea	22.29	21.40
1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)	26.28	24.04
1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene	27.48	29.69
1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene)	23.34	22.91
1,1'-(2,2-dichloroethylidenebis(4-chlorobenzene)	27.31	22.15
1,1-(di-p-chlorophenyl)-2-nitropropane	21.39	23.23
1,1,1,3-tetrachloropropane	12.69	17.85
1,1,1-trichloro-3,3,3-trifluoropropane	14.07	13.70
1,1,1-trichloroethane	10.13	9.87
1,1,1-trifluoro-3,3-dichloropropane	10.33	11.81
1,1,1-trifluoro-3-chloropropane	9.80	12.40
1,1,1-trifluoroethane	6.19	4.41
1,1,1-trifluoro-n-[2-methyl-4-(phenylsulphonyl)phenyl] methane sulfonamide	31.79	27.67
1,1,1-trinitroethane	16.32	13.33
1,1,2,2-tetrachlorodifluoroethane	5.52	12.57
1,1,2,2-tetrachloroethane	9.72	12.43
1,1,2-tribromoethane	9.11	10.11

1,1,2-trichloroethane	11.38	13.02
1,1,2-trifluoro-1,2,2-trichloroethane	4.86	10.75
1,1,3,3-tetraethylurea	20.55	25.67
1,1,3-trimethylurea	14.30	19.70
1,10-decanediol	41.70	39.91
1,12-benzoperylene	17.37	20.83
1,1-bis(4-chlorophenyl)-2-nitrobutane	15.41	26.18
1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene	23.55	16.88
1,1-dichloroethane	7.87	7.98
1,1-dichloroethene	6.51	6.91
1,1-dicyclohexyldodecane	44.35	53.91
1,1-diethylurea	20.37	26.85
1,1-difluoro-1-chloroethane	2.69	6.23
1,1-dimethyl-3-phenylurea	22.81	25.03
1,1-dimethylcyclohexane	11.37	13.24
1,1-dimethylcyclopentane	10.09	10.91
1,1-dimethylurea	29.11	20.96
1,1-diphenyldodecane	41.68	45.12
1,2,3,4,5,6,7,8-octahydroanthracene	20.86	22.52
1,2,3,4,5-pentahydroxypentane (D-Arabitol)	38.90	30.38
1,2,3,4,5-pentahydroxypentane (Ribitol)	37.60	30.38
1,2,3,4,5-pentahydroxypentane (Xylitol)	37.40	30.38
1,2,3,4-tetracarbomethoxybenzene	40.40	30.98
1,2,3,4-tetracarbomethoxynaphthalene	35.90	34.51
1,2,3,4-tetrachlorobenzene	17.00	13.65
1,2,3,4-tetrafluorobenzene	10.93	9.62
1,2,3,4-tetrahydronaphthlene	12.45	16.03
1,2,3,4-tetrahydroquinoline	11.81	17.08
1,2,3,4-tetrahydroxybutane	42.36	25.50
1,2,3,4-tetramethylbenzene	11.23	12.70
1,2,3,5-tetracarbomethoxybenzene	32.60	30.98
1,2,3,5-tetrachlorobenzene	19.00	13.65
1,2,3,5-tetrafluorobenzene	10.67	9.62
1,2,3,5-tetramethylbenzene	12.93	12.70
1,2,3,6,7,8-hexahydropyrene	23.52	21.39
1,2,3-tribromopropane	23.78	19.44
1,2,3-tricarbomethoxybenzene	32.70	27.02
1,2,3-tricarbomethoxynaphthalene	23.70	29.15
1,2,3-trichlorobenzene	20.50	12.62
1,2,3-trihydroxybenzene	18.55	20.66
1,2,3-trihydroxypropane	18.28	21.06
1,2,3-trimethylbenzene	10.17	11.91
1,2,4,5,8,9-tribenzopyrene	28.80	27.54
1,2,4,5-tetrabromobenzene	28.22	17.60
1,2,4,5-tetracarbomethoxybenzene	35.70	30.98
1,2,4,5-tetracarbomethoxynaphthalene	36.40	34.51
1,2,4,5-tetrachloro-3-nitrobenzene	19.46	17.09
1,2,4,5-tetrachlorobenzene	24.10	13.65
1,2,4,5-tetrafluorobenzene	15.05	9.62
1,2,4,5-tetramethylbenzene	20.88	12.70
1,2,4-triazole	16.10	17.52
1,2,4-tricarbomethoxynaphthalene	32.10	29.15
1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene	28.94	22.50

1,2,4-trimethylbenzene	13.19	11.91
1,2,5,6-tetracarbomethoxynaphthalene	42.10	34.51
1,2,5-tricarbomethoxynaphthalene	25.50	29.15
1,2,6,7-tetracarbomethoxynaphthalene	34.20	34.51
1,2,6-tricarbomethoxynaphthalene	35.90	29.15
1,2,7,8-tetrahydroxyoctane	36.70	37.49
1,2,7-tricarbomethoxynaphthalene	36.10	29.15
1,2,8-tricarbomethoxynaphthalene	24.80	29.15
1,2:3,4-dibenzanthracene	25.82	23.65
1,2:3,4-dibenzopyrene	24.68	24.01
1,2:4,5-dibenzopyrene	30.50	24.01
1,2:5,6-dibenzanthracene	31.16	23.65
1,2-benzacenaphthene (fluoranthene)	18.74	16.95
1,2-benzanthracene	21.38	20.12
1,2-benzofluorene	22.20	19.04
1,2-benzopyrene	19.08	20.48
1,2-bromochlorobenzene	12.37	12.58
1,2-bromoiodobenzene	14.42	14.53
1,2-butadiene	6.95	4.33
1,2-chloronitrobenzene	19.08	14.00
1,2-diamino-2-methylpropane	18.90	15.35
1,2-diaminopropane	18.49	15.55
1,2-dibenzoylethane	39.58	25.13
1,2-dibromo-1,1-difluoroethane	8.30	12.91
1,2-dibromobenzene	12.61	13.57
1,2-dibromoethane	13.14	15.24
1,2-dibromotetrafluoroethane	7.04	10.57
1,2-dicarbomethoxybenzene	16.95	20.26
1,2-dicarbomethoxynaphthalene	27.60	23.79
1,2-dichlorobenzene	12.93	11.59
1,2-dichloroethane	8.83	13.60
1,2-dichloropropane	6.40	11.94
1,2-dichloro-tetrafluoroethane	7.04	8.93
1,2-dicyanobenzene	20.00	17.80
1,2-difluoro-2,2-dichloroethane	8.19	11.27
1,2-difluorobenzene	11.05	9.58
1,2-dihydro-6-neopentyl-2-oxonicotinic acid	19.33	26.92
1,2-dihydroxybenzene	22.01	16.57
1,2-diiodobenzene	14.01	15.50
1,2'-dinaphthylmethane	30.54	23.32
1,2-dinitrobenzene	22.84	16.40
1,2-diphenyl-2-(N-piperidinyl)-1-ethanone	33.93	29.25
1,2-diphenylethane	25.40	18.36
1,2-pentadiene	7.56	4.95
1,3,3-trinitroazetidine	30.31	20.56
1,3,5,5-tetranitro-1,3-diazacyclohexane	29.37	31.00
1,3,5,7-tetroxane	22.59	26.60
1,3,5-tri-a-naphthylbenzene	42.26	35.70
1,3,5-tricarbomethoxynaphthalene	25.90	29.15
1,3,5-trichloro-2,4,6-trifluorobenzene	19.83	12.69
1,3,5-trichlorobenzene	18.20	12.62
1,3,5-trimethylbenzene	9.51	11.91
1,3,5-trinitro-1,3,5-triazacyclohexane	37.66	31.31

1,3,5-trinitrobenzene	16.71	19.84
1,3,5-trinitroso-1,3,5-triazacyclohexane	21.98	28.49
1,3,5-trioxane	15.11	19.95
1,3,5-triphenylbenzene	33.40	25.11
1,3,6-trimethyluracil	21.20	18.74
1,3,7-tricarbomethoxynaphthalene	37.20	29.15
1,3,7-trichlorodibenzodioxin	30.80	19.87
1,3,8-tricarbomethoxynaphthalene	27.70	29.15
1,3-bromochlorobenzene	12.29	12.58
1,3-bromoiodobenzene	12.16	14.53
1,3-butadiene	7.98	7.94
1,3-cyclohexadiene	4.20	10.80
1,3-dibromobenzene	13.21	13.57
1,3-dibromopropane	14.64	18.19
1,3-dibutylurea	27.23	38.79
1,3-dicarbomethoxybenzene	25.30	20.26
1,3-dicarbomethoxynaphthalene	30.50	23.79
1,3-dichlorobenzene	12.64	11.59
1,3-dicyanopropane	12.59	19.33
1,3-diethylurea	14.33	26.99
1,3-difluorobenzene	9.40	9.58
1,3-dihydroxybenzene	20.10	16.95
1,3-diiodobenzene	15.93	15.50
1,3-dimethyluracil	14.60	16.57
1,3-dimethylurea	13.90	21.09
1,3-dinitro-1,3-diazacycloheptane	24.90	29.10
1,3-dinitro-1,3-diazacyclohexane	19.28	25.53
1,3-dinitro-1,3-diazacyclopentane	25.54	24.44
1,3-dinitro-5-nitroso-1,3,5-triazacyclohexane	25.97	30.37
1,3-dinitrobenzene	17.36	16.40
1,3-dioxolane	9.87	15.63
1,3-diphenylacetone	20.20	20.70
1,3-diphenylurea	34.60	31.74
1,3-dithiane	15.20	22.90
1,3-nitrochlorobenzene	19.37	14.00
1,4,5,8-tetracarbomethoxynaphthalene	36.10	34.51
1,4,5-tricarbomethoxynaphthalene	26.50	29.15
1,4,6-tricarbomethoxynaphthalene	30.20	29.15
1,4-[bis[(4-methylphenyl)amino]-9,10-anthracenedione	36.59	32.55
1,4-bis(diphenylphosphino)butane	45.30	49.43
1,4-bis(phenylglyoxaloyl)benzene	32.30	32.50
1,4-bis-[4-(4'-n-butylbiphenyl)]butane	37.74	49.26
1,4-bromochlorobenzene	18.76	12.58
1,4-bromoiodobenzene	19.13	14.53
1,4-cyclohexadiene	6.53	10.80
1,4-cyclohexanedione	17.15	17.87
1,4-diamino-2-methoxyanthraquinone	35.29	31.56
1,4-diaminoanthraquinone	24.20	27.71
1,4-dibromobenzene	20.04	13.57
1,4-dicarbomethoxybenzene	32.09	20.26
1,4-dicarbomethoxynaphthalene	20.40	23.79
1,4-dichloro-2,5-dimethoxybenzene	27.56	19.30
1,4-dichlorobenzene	18.16	11.59

1,4-dihydroxybenzene	26.95	16.95
1,4-dihydroxybutane	18.70	22.22
1,4-diiodobenzene	22.37	15.50
1,4-dimethylnaphthalene	10.60	14.65
1,4-dinitrobenzene	28.12	16.40
1,4-dioxane	15.20	17.96
1,4-dioxane-2,5-dione	16.87	18.97
1,4-di-tert-butylbenzene	22.48	16.06
1,4-dithiane	21.60	22.90
1,4-nitrochlorobenzene	11.85	14.00
1,4-pentadiene	6.14	3.35
1,5-cyclooctanedione	11.92	22.53
1,5-dicarbomethoxynaphthalene	26.40	23.79
1,5-dichloro-3-oxapentane	8.39	21.07
1,5-dimethyltetrazole	14.70	13.65
1,5-dinitro-3-nitroso-1,3,5-triazacycloheptane	30.89	32.70
1,5-pentanediol	15.72	25.17
1,6-bis-[4-(4'-ethylbiphenyl)]hexane	38.90	45.08
1,6-dicarbomethoxynaphthalene	22.10	23.79
1,6-hexanediol	25.05	28.11
1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane	38.49	50.67
1,7-dicarbomethoxynaphthalene	20.00	23.79
1,7-heptanediol	21.30	31.06
1,8-bis-(4-biphenyl)octane	56.00	46.44
1,8-bis-[4-(4'-ethylbiphenyl)]butane	46.00	37.46
1,8-bis-[4-(4'-ethylbiphenyl)]octane	50.40	49.26
1,8-bis-[4-(4'-n-butylbiphenyl)]octane	40.00	61.06
1,8-dimethylnaphthalene	15.77	14.65
1,8-octanediol	36.10	34.01
1,9-nonanediol	36.40	36.96
10H-phenothiazine	26.92	24.89
10-nonadecanone	66.67	51.35
10-octadecynoic acid	52.32	47.21
11-cyclohexyleicosane	48.70	64.75
11-heneicosanone	76.20	57.25
11-n-decylheneicosane	71.13	84.44
11-octadecynoic acid	55.97	47.21
11-phenyleicosane	64.77	61.41
12-octadecynoic acid	49.79	47.21
12-tricosanone	78.03	63.15
13-octadecynoic acid	55.51	47.21
14-octadecynoic acid	52.74	47.21
16-octadecynoic acid	60.10	49.55
17-octadecynoic acid	54.20	55.29
1-8-naphthalic anhydride	23.32	20.16
1a,2a,3ß,4a,5a,6ß-hexachlorocyclohexane	22.13	22.60
1-acetoxynaphthalene	20.21	17.89
1-acetyl-2-naphthol	21.34	19.65
1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione	30.79	34.01
1-aminoanthraquinone	28.78	25.49
1-aminopropane	10.97	11.80
1-benzoyl-2-naphthol	31.35	20.49
1-bromo-2-chloro-1,1,2-trifluoroethane	4.38	9.68

1-bromo-2-chloroethane	14.02	14.42
1-bromobutane	9.23	15.28
1-bromodocosane	68.12	68.36
1-bromoheptane	21.76	24.13
1-bromohexane	18.05	21.18
1-bromonaphthalene	15.16	15.08
1-bromononane	30.12	30.02
1-bromooctane	24.69	27.07
1-bromopentane	14.37	18.23
1-bromotricosane	103.34	91.95
1-bromoundecane	33.47	35.92
1-butene	3.85	4.49
1-butyne	6.03	6.71
1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene	23.09	24.04
1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene	23.84	16.88
1-chloro-2,2-(bis-(4-chlorophenyl)ethylene	25.52	15.35
1-chlorodibenzodioxin	23.20	17.81
1-chloronaphthalene	12.90	14.09
1-cis-3-pentadiene	5.64	9.21
1-cyclohexyl-1-phenyldodecane	35.19	50.57
1-decanethiol	33.30	30.15
1-decanol	37.66	33.51
1-decene	22.10	22.18
1-deoxy-D-glucopyranose	27.40	29.94
1-docosanol	63.80	68.90
1H-1,2,4-triazol-3-amine	21.93	21.04
1-heptanethiol	25.40	21.30
1-heptanol	18.16	24.67
1-heptene	12.64	13.34
1-hexacosanol	84.52	80.70
1-hexadecanol	58.41	51.21
1-hexadecene	34.08	39.88
1-hexanethiol	18.03	18.35
1-hexanol	15.48	21.72
1-hexene	9.35	10.39
1-iodonaphthalene	15.91	16.05
1-methoxy-2-(2,2,2-tricloro-1-(4-methoxyphenyl)ethyl)benzene	22.45	29.69
1-methyl-7-isopropylphenanthrene	18.03	19.13
1-methyl-9H-pyrido[3,4-b]indole	27.20	23.29
1-methylcyclohexanol	10.87	15.73
1-methylcyclopentanol	8.41	13.40
1-methylnaphthalene	11.97	13.86
1-methyltetrazole	15.70	12.86
1-naphthaleneacetamide	32.82	25.63
1-naphthaleneacetic acid	22.26	22.61
1-naphthoic acid	19.89	22.77
1-naphthyl benzoate	16.98	23.75
1-naphthyl methylcarbamate	24.51	24.86
1-naphthylamine	15.53	16.58
1-nitronaphthalene	18.43	16.50
1-nonanethiol	33.50	27.20
1-nonene	19.97	19.24
1-octanethiol	24.27	24.25

1-octene	15.31	16.29
1-pentadecanol	54.73	48.26
1-pentanethiol	17.53	15.40
1-pentanol	10.50	18.77
1-pentene	5.81	7.44
1-propanethiol	9.95	9.51
1-propanol	5.37	12.87
1-tetradecanol	49.37	45.31
1-undecene	26.48	25.13
2-((4-chloro-6-(cyclopropylamino)-1,3,5-triazin-2-yl)amino-2-methylpropanenitrile	22.51	37.12
2-(1,3-dioxolan-2-yl)phenyl methylcarbamate	23.82	32.09
2-(1'-cyclohexenyl)cyclohexanone	17.26	23.91
2-(1-methylethyl)phenyl methylcarbamate	26.14	23.07
2-(2,4,5-trichlorophenoxy)propanoic acid	39.58	27.06
2-(2,4-dichlorophenoxy)propanoic acid	30.43	26.03
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	29.50	22.74
2-(3-hydroxy-2-quinolinyl)-1H-indene-1,3(2H)-dione	30.89	28.23
2-(4-chloro-2-methylphenoxy)propanoic acid	26.43	25.79
2-(6-methoxy-2-naphthyl)propionic acid	29.41	25.84
2-(dimethylamino)-1,2-diphenylethanone	22.38	22.03
2-(docosanoxy)ethanol	56.85	76.37
2-(hexadecyloxy)ethanol	52.26	58.67
2,11-dicyclohexyldodecane	43.93	49.31
2,2,2-trinitroethanol	22.59	19.73
2,2,2-trinitroethyl 4,4,4-trinitrobutyrate	32.64	39.61
2,2,2-trinitroethyl-4,4-dinitropentanoate	26.78	35.98
2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	22.60	23.99
2,2',3,3',5,5',6,6'-octachlorobiphenyl	22.80	22.96
2,2',3,3',5,5',6-heptachlorobiphenyl	20.30	21.93
2,2',3,3',5,5'-hexachlorobiphenyl	29.20	20.90
2,2',3,3',6,6'-hexachlorobiphenyl	21.10	20.90
2,2,3,3-tetramethylbutane	12.44	12.95
2,2,3,3-tetramethylpentane	13.41	15.90
2,2,3-trimethylbutane	7.07	9.53
2,2',4,4',6,6'-hexachlorobiphenyl	17.50	20.90
2,2,4,4-tetramethylpentan-3-ol	9.63	17.64
2,2,4,4-tetramethylpentane	9.75	15.90
2,2',4,5,5'-pentachlorobiphenyl	18.80	19.87
2,2',4',5-tetrachlorobiphenyl	23.40	18.84
2,2,4-trimethylpentane	9.20	12.48
2,2,5,5-tetramethylhex-3-ene	16.41	10.09
2,2,6,6-tetramethyl-1,3-dioxane	10.90	16.49
2,2-bis-(4-cyanatophenyl)propane	26.69	25.67
2,2-bis(phenylthio)propane	24.40	27.07
2,2-bis-hydroxymethylpropanoic acid	45.89	28.42
2,2-dichloropropane	9.91	11.40
2,2-dicyanopropane	13.92	12.69
2,2-dimethoxy-1,2-diphenylethanone	20.86	21.19
2,2-dimethyl-1,3-dioxan	12.10	17.22
2,2-dimethyl-1,3-propanediol	22.25	21.03
2,2-dimethyl-1-propanol	8.21	14.63
2,2-dimethylbutane	8.00	11.18

2,2-dimethylheptane	12.18	20.03
2,2-dimethylpentane	5.86	14.13
2,2-dimethylpropane	7.98	8.24
2,2-dimethylpropanoic acid (pivalic acid)	11.36	15.62
2,2-dinitro-1,3-propanediol	21.34	23.02
2,2-dinitropropane	18.55	10.23
2,2-dinitropropanol	22.44	16.63
2,2-dinitropropyl-4,4-dinitropentanoate	32.09	32.88
2,2-dintropropyl-4,4,4-trinitrobutyrate	63.26	32.06
2,2'-methylenebis(3,4,6-trichlorophenol)	33.26	29.47
2,3,4,5,6-pentachlorobiphenyl	21.35	19.87
2,3,4,5,6-pentafluorotoluene	13.28	10.44
2,3,4,5-tetrachlorobiphenyl	25.20	18.84
2,3,4-trimethylpentane	9.27	7.40
2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione	30.87	23.32
2,3,5-tricarbomethoxynaphthalene	41.00	29.15
2,3,5-triiodobenzoic acid	32.23	26.89
2,3,6,7,10,11-hexakis(1-decynyl)triphenylene	63.00	129.05
2,3,6,7-tetracarbomethoxynaphthalene	42.20	34.51
2,3,6-tricarbomethoxynaphthalene	34.40	29.15
2,3,6-trichlorobenzoic acid	23.85	19.73
2,3,6-trichlorophenylacetic acid	22.43	22.17
2,3-benzofluorene	23.40	19.04
2,3-dicarbomethoxynaphthalene	20.20	23.79
2,3-dichloro-1,4-naphthalenedione	28.53	21.80
2,3-dichlorophenol	21.36	15.11
2,3-dihydro-2,2-dimethyl-7-benzofuranol-3-one	21.79	20.61
2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	30.33	26.74
2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	26.66	27.48
2,3-dimethyl-2,3-bis(4-tert-butylphenyl)butane	43.93	28.60
2,3-dimethyl-2,3-bis(phenylazo)butane	21.09	25.33
2,3-dimethyl-2,3-butanediol	14.70	17.92
2,3-dimethyl-2,3-diphenylbutane	25.52	22.07
2,3-dimethyl-2-butene	9.97	9.76
2,3-dimethylbenzoic acid	18.30	20.82
2,3-dimethylbutane	7.69	6.11
2,3-dimethylnaphthalene	15.90	14.65
2,3-dimethylphenol	21.02	14.83
2,3-dimethylpyridine	13.48	11.92
2,3-dinitrophenol	26.24	18.82
2,3-dinitrotoluene	17.57	17.20
2,3-pentadiene	6.61	5.60
2,4,4-trimethyl-1-pentene	8.79	11.51
2,4,4-trimethyl-2-pentene	6.78	9.93
2,4,5,6-tetrachloro-1,3-benzenedicarbonitile	30.00	21.92
2,4,5-tribromostyrene	25.10	17.10
2,4,5-trichlorobiphenyl	22.80	17.81
2,4,5-trichlorophenol	21.59	16.14
2,4,5-trimethylthiazole	9.00	12.73
2,4,5-trinitrotoluene	24.70	20.63
2,4,6,N-tetranitro-N-methyltoluidene	19.33	24.61
2,4,6-N-tetranitroethylaniline	23.51	30.21
2,4,6-tribromophenol	18.52	18.91

2,4,6-trichlorobiphenyl	16.50	17.81
2,4,6-trimethyl-1,3,5-trioxane	15.53	17.99
2,4,6-trimethylpyridine	9.54	12.71
2,4,6-trinitro-1,3-dimethylbenzene	38.49	21.42
2,4,6-trinitroresorcinol	33.50	22.08
2,4,6-trinitrotoluene	23.43	20.63
2,4,6-tri-tert-butylphenol	19.46	23.04
2,4,7-trinitrofluoren-9-one	26.40	28.65
2,4-dibromophenol	14.64	17.08
2,4-dichlorophenol	20.09	15.11
2,4-dichlorophenyl 4-nitrophenyl ether	22.96	21.33
2,4-dimethylpentane	6.85	9.06
2,4-dimethylpyridine	8.82	11.92
2,4-dimethylpyrrole	9.60	16.22
2,4-dimethylthiazole	2.90	11.94
2,4-dinitrochlorobenzene	20.17	17.43
2,4-dinitrophenol	24.17	18.82
2,4-dinitrotoluene	20.12	17.20
2,4-di-tert-butylthiazole	10.50	16.88
2,4-hexadiyne	2.90	4.59
2,5,8,11-tetraoxadodecane	23.71	27.49
2,5,8-trioxanonane	17.78	20.03
2,5-dibutoxy-1,4-benzoquinone	41.27	41.61
2,5-dichlorophenol	22.43	15.11
2,5-diethoxy-1,4-benzoquinone	28.70	29.82
2,5-dimethylaniline	13.70	14.63
2,5-dimethylphenol	23.38	14.83
2,5-dimethylpyridine	14.64	11.92
2,5-dimethylpyrrole	9.30	16.22
2,5-dimethyltetrazole	13.50	13.65
2,5-dimethylthiophene	8.91	11.13
2,5-di-n-heptadecyloxy-1,4-benzoquinone	133.90	119.03
2,5-di-n-heptyloxy-1,4-benzoquinone	59.30	60.05
2,5-di-n-hexadecyloxy-1,4-benzoquinone	122.90	113.13
2,5-di-n-hexyloxy-1,4-benzoquinone	45.45	53.41
2,5-dinitrophenol	23.73	18.82
2,5-di-n-nonadecyloxy-1,4-benzoquinone	150.20	130.83
2,5-di-n-nonyloxy-1,4-benzoquinone	79.30	71.85
2,5-di-n-octyloxy-1,4-benzoquinone	52.40	65.95
2,5-di-n-pentadecyloxy-1,4-benzoquinone	123.40	107.23
2,5-di-n-undecyloxy-1,4-benzoquinone	93.40	83.64
2,5-dipentoxy-1,4-benzoquinone	47.68	47.51
2,5-dipropoxy-1,4-benzoquinone	44.70	35.72
2,6-dichloro-4-benzenamine	29.48	15.11
2,6-dichloro-4-nitroaniline	32.64	18.16
2,6-dichlorobenzonitrile	26.17	15.73
2,6-dichlorobiphenyl	12.60	16.78
2,6-dichlorophenol	22.14	14.92
2,6-diisopropylphenol	14.64	16.74
2,6-dimethylnaphthalene	25.06	14.65
2,6-dimethylphenol	18.90	14.83
2,6-dimethylpyridine	13.04	11.92
2,6-dinitrochlorobenzene	18.95	17.43

2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	22.32	30.38
2,6-dinitrophenol	19.58	17.52
2,6-dinitrotoluene	23.85	17.20
2,6-di-tert-butyl-4-methoxyphenol	26.90	23.63
2,6-di-tert-butyl-4-methylphenol	23.85	20.56
2,6-di-tert-butylphenol	16.57	19.77
2,7-dicarbomethoxynaphthalene	26.60	23.79
2,7-dimethylnaphthalene	23.35	14.65
2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	35.49	24.48
2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	38.00	28.42
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	41.96	37.26
2-[bis(2-chloroethyl)amino]tetrahydro-2H-1,3,2-oxazophosphorine-2-oxide	33.13	31.61
2-acetoxynaphthalene	20.05	17.89
2-acetyl-1-naphthol	22.52	20.95
2-acetylamino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	53.83	47.04
2-acetylamino-9-[(2-hydroxyethoxy)methyl]-9H-purine	54.92	41.39
2-amino-2-hydroxymethylpropane-1,3-diol	35.64	29.21
2-amino-2-methylpropane-1,3-diol	30.49	22.81
2-amino-9-[(2-acetoxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	49.90	40.69
2-amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	30.44	38.62
2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	42.20	32.98
2-aminobenzoic acid	20.50	20.16
2-aminobiphenyl	13.99	18.24
2-aminopropane	7.33	7.20
2-benzoyl-1-naphthol	20.18	21.79
2-bromo-2-chloro-1,1,1-trifluoroethane	4.84	9.68
2-bromobutane	6.88	10.67
2-bromonaphthalene	20.35	15.08
2-bromopropane	6.55	7.72
2-bromothiophene	7.92	11.56
2-butanethiol	6.48	7.85
2-butanol	5.97	11.16
2-butanone	8.44	9.45
2-butyne	9.25	3.30
2-carbomethoxynaphthalene	27.10	18.43
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	30.07	26.54
2-chloro-2-nitropropane	13.01	12.67
2-chloro-6-(trichloromethyl)pyridine	20.30	16.26
2-chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene	27.82	23.11
2-chloroanthraquinone	39.00	24.30
2-chlorobenzoic acid	25.73	18.97
2-chlorobiphenyl	14.54	15.76
2-chlorodibenzodioxin	23.10	17.81
2-chloroethylphosphonic acid	14.79	19.96
2-chloro-n-(2,6-diethylphenyl)-n-(methoxymethyl)acetamide	25.31	25.64
2-chloronaphthalene	14.70	14.09
2-chloro-N-isopropyl N-phenylacetamide	26.05	19.59
2-chloro-N-isopropylacetamide	26.05	20.14
2-chlorophenol	12.61	14.08
2-chloropropane	7.39	6.90
2-chlorothiophene	8.97	10.58

2-cyano-2-methylpropane	11.43	11.81
2-cyclohexyl-4,6-dinitrophenol	28.03	27.93
2-cyclohexylcyclohexanone	18.00	25.08
2-deoxy-2-fluoro-D-glucopyranose	38.20	29.56
2-deoxy-D-glucopyranose	34.50	29.94
2-ethoxyisonitrosoacetanilide	23.00	35.59
2-ethyl-2-diphenylmethyl-1,3-cyclopentanedione	28.20	29.87
2-fluorenyl-2-methyl-1,3-cyclohexanedione	35.70	24.91
2-fluorenyl-2-methyl-1,3-cyclopentanedione	24.60	22.58
2-fluorotoluene	9.80	10.35
2-heneicosanone	77.65	59.58
2-heptanone	19.71	18.30
2-hexadecanoyloxy-1,3-bis-(9-cis-octadecenoyloxy)propane	125.50	138.04
2-hexanone	14.90	15.35
2-hydroxybenzoic acid	24.60	20.35
2-hydroxymethyl-2-methyl-1,3-propanediol	36.15	27.43
2-iodobenzoic acid	21.38	20.92
2-iodonaphthalene	16.04	16.05
2-isopropoxyphenyl N-methylcarbamate	22.96	26.47
2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide	16.92	17.30
2-methyl-1,3-butadiene	4.92	6.91
2-methyl-1-butene	7.91	6.80
2-methyl-1-phenyl-2-(N-piperidinyl)-1-propanone	16.74	26.41
2-methyl-1-propanol	6.32	11.21
2-methyl-2-(methylsulfonyl)propanal oxime	27.12	21.45
2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime	22.71	29.44
2-methyl-2-butanethiol	7.67	10.80
2-methyl-2-butanol	8.21	13.67
2-methyl-2-butene	7.59	7.45
2-methyl-2-diphenylmethyl-1,3-cyclopentanedione	34.30	26.92
2-methyl-2-nitro-1,3-propandiol	34.83	23.37
2-methyl-2-nitro-1-propanol	23.76	16.97
2-methyl-2-nitropropyl-4,4,4-trinitrobutyrate	29.96	32.41
2-methyl-4,6-dinitrophenol	19.41	19.61
2-methylbutane	5.13	6.91
2-methylcyclothiapentane	8.87	15.46
2-methyldecane	25.06	25.46
2-methylfuran	8.55	9.69
2-methylheptane	11.92	16.61
2-methylhexane	9.18	13.66
2-methylnaphthalene	18.11	13.86
2-methylnonane	17.49	22.51
2-methylpentane	6.27	10.71
2-methylpiperidine	18.58	14.37
2-methylpyridine	9.72	11.13
2-methyltetrazole	12.37	12.86
2-methylthiazole	12.16	11.14
2-methylthiophene	9.47	10.34
2-naphthoic acid	23.54	22.77
2-naphthyl benzoate	26.23	23.75
2-naphthylamine	23.33	16.58
2-n-butyl-5-(4-bromobiphenyl-4-yl)thiophene	21.40	29.26
2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	18.44	22.14

2-nitro-5-methylphenol	20.79	16.18
2-nitroaniline	16.11	15.19
2-nonadecanone	68.65	53.69
2-n-propyl-5-(4-bromophenyl)thiophene	15.70	26.31
2-octanone	24.42	21.25
2-pentadecanone	54.39	41.89
2-pentanol	8.48	14.11
2-pentanone	11.06	12.40
2-phenylbenzimidazole	22.18	24.16
2-piperadone	16.10	23.37
2-propanethiol	5.78	4.90
2-propanol	5.41	8.21
2-pyrrolidone	13.92	21.04
2-sec-butyl-4,6-dinitrophenol	21.81	22.22
2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate	18.89	32.25
2-tetradecanone	49.12	38.94
2-undecanone	28.78	30.09
3-(1-methylethyl)-(1H)-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide	21.77	22.15
3-(3,4-dichlorophenyl)-1,1-dimethylurea	33.89	27.08
3-(4-chlorophenyl)-1,1-dimethylurea	29.46	26.06
3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	25.46	24.22
3(n-decylamino)-1,2-propanediol	54.80	48.81
3(n-decyloxy)-1,2-propanediol	38.90	45.67
3(n-decylthio)-1,2-propanediol	34.60	46.91
3(n-dodecylamino)-1,2-propanediol	62.10	54.71
3(n-dodecyloxy)-1,2-propanediol	51.40	51.57
3(n-dodecylthio)-1,2-propanediol	38.40	52.81
3(n-heptylamino)-1,2-propanediol	28.80	39.96
3(n-heptyloxy)-1,2-propanediol	25.62	36.82
3(n-heptylthio)-1,2-propanediol	29.28	38.06
3(n-hexyloxy)-1,2-propanediol	10.20	33.87
3(n-hexylthio)-1,2-propanediol	48.50	35.11
3(n-nonylamino)-1,2-propanediol	53.20	45.86
3-(n-nonyloxy)-1,2-propanediol	29.50	42.72
3(n-octylamino)-1,2-propanediol	45.10	42.91
3(n-octyloxy)-1,2-propanediol	33.40	39.77
3(n-octylthio)-1,2-propanediol	39.80	41.01
3(n-tetradecylamino)-1,2-propanediol	64.90	60.61
3(n-tetradecyloxy)-1,2-propanediol	62.10	57.46
3(n-tetradecylthio)-1,2-propanediol	43.10	58.71
3(n-tridecylamino)-1,2-propanediol	68.70	57.66
3(n-tridecyloxy)-1,2-propanediol	51.40	54.51
3(n-tridecylthio)-1,2-propanediol	34.00	55.76
3(n-undecylamino)-1,2-propanediol	58.20	51.76
3(n-undecyloxy)-1,2-propanediol	43.10	48.62
3(n-undecylthio)-1,2-propanediol	30.30	49.86
3-(p-tolyl-4-sulfonyl)-1-butyl urea	25.61	33.20
3,3',4'4'-tetraaminodiphenyl ether	26.71	29.13
3,3',5,5'-tetra-tert-butyldiphenylmethane-4,4'-diol	42.97	36.73
3,3'-bis-(1-cyclohexylethyl)-5,5'-dimethyldiphenylmethane-2,2'-diol	29.29	53.59
3,3-bis-(chloromethyl)oxacyclobutane	16.95	20.65
3,3-diethylpentane	11.57	20.03

3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime	19.83	26.73
3,3-dimethyl-1-butene	6.61	6.35
3,3-dimethyl-2-butanone	11.34	11.31
3,3-dimethylpentane	7.07	14.13
3,3-dimethylpentanedioic anhydride	17.99	16.17
3,3'-di-tert-butyl-5,5'-dimethyl-2,2-dihydroxydiphenylmethane	29.33	31.79
3,4-benzophenanthrene	16.32	20.12
3,4-benzopyrene	27.21	20.48
3,4-dichloro-2-methoxybenzoic acid	35.33	23.66
3,4-dichlorophenol	20.93	15.30
3',4'-dichloropropionanilide	18.26	24.14
3,4-diethyl-3,4-bis(4-tert-butylphenyl)hexane	29.71	40.40
3,4-dimethylisoxazol 5-sulphanylamide	28.01	26.85
3,4-dimethylphenol	18.13	14.83
3,4-dimethylphenyl methylcarbamate	24.97	22.91
3,4-dimethylpyridine	14.70	11.92
3,4-dinitrophenol	25.37	20.11
3,4-dinitrotoluene	18.83	17.20
3,5,6-trichloro-2-pyridinol	25.79	16.94
3,5,6-trichloro-2-pyridinyloxyacetic acid	31.17	27.53
3,5-dibromo-4-hydroxybenzonitrile	32.03	21.03
3,5-dichlorobenzoic acid	22.97	21.29
3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	28.68	26.53
3,5-dichlorophenol	20.51	15.30
3,5-diisopropylphenol	12.13	16.74
3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate	18.37	25.65
3,5-dimethylbenzoic acid	22.60	20.82
3,5-dimethylphenol	18.00	14.83
3,5-dimethylpyridine	13.11	11.92
3,5-dinitrobenzoic acid	22.80	26.11
3,6-dichloro-2-methoxybenzoic acid	22.90	23.66
3,6-dichloro-5-hydroxy-2-methoxybenzoic acid	28.98	26.08
3-amino-2,5-dichlorobenzoic acid	37.42	23.32
3-aminoacetophenone	29.00	17.22
3-aminobenzoic acid	21.84	22.75
3-bromopentane	8.40	13.62
3-chloro-1,1,1,3,3-pentafluoropropane	10.47	10.06
3-chlorobenzoic acid	23.85	20.26
3-chlorophenol	14.91	14.27
3-deoxy-3-fluoro-D-glucopyranose	18.30	29.56
3-deoxy-D-glucopyranose	32.60	29.94
3-diphenylmethyl-2,4-pentanedione	27.02	24.76
3-ethyl-3-diphenylmethyl-2,4-pentanedione	34.70	26.75
3-ethylheptane	16.02	19.56
3-ethylpentane	9.55	13.66
3-fluorotoluene	8.30	10.35
3-heptanone	17.53	15.97
3-hexanone	14.50	13.02
3-hydroxybenzoic acid	26.20	22.94
3-iodobenzoic acid	28.70	22.22
3-methyl-1,2-butadiene	7.95	6.64
3-methyl-1-butanethiol	7.41	10.80
3-methyl-1-butene	5.36	4.83

3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	21.39	24.40
3-methyl-2-butanethiol	7.67	6.19
3-methyl-3-diphenylmethyl-2,4-pentanedione	25.10	23.80
3-methylcyclothiapentane	10.37	15.46
3-methylheptane	11.67	16.61
3-methylpentane	5.31	10.71
3-methylpyridine	14.18	11.13
3-methylthiophene	10.54	10.34
3-nitroaniline	23.68	16.48
3-nitrophthalic anhydride	18.40	20.06
3-nitrotoluene	14.98	13.76
3-pentanol	9.08	14.11
3-pentanone	11.71	10.07
3-propyl-3-diphenylmethyl-2,4-pentanedione	27.10	29.70
4-(1,1-dimethylethyl)-n-(1-methylpropyl)-2,6-dinitrobenzeneamine	20.84	26.77
4-(2,4,5-trichlorophenoxy)butanoic acid	30.28	32.62
4-(2,4-dichlorophenoxy)butyric acid	38.42	31.59
4-(2-chlorophenylhydrazone)-3-methyl-5-isoxazolone	28.04	26.90
4-(4-chloro-2-methylphenoxy)butanoic acid	32.02	31.35
4-(4-nitrophenylazo)aniline	31.88	22.75
4-(6-hexenyloxy)-3',4'difluorodiphenyldiacetylene	37.45	30.47
4-(cis-3-hexenyloxy)-3',4'difluorodiphenyldiacetylene	30.97	26.46
4-(cis-4-hexenyloxy)-3',4'difluorodiphenyldiacetylene	35.32	28.79
4-(dipropylamino)-N,N-dimethyl-3,5-dinitrobenzenesulfonamide	32.57	38.06
4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide	38.48	33.15
4,4'-di-(2-methoxyethoxy)biphenyl	40.20	37.37
4,4'dichlorodiphenylsulphone	24.40	20.44
4,4'-didecanoyloxydiphenyldiacetylene	87.10	68.93
4,4'-didodecanoyloxydiphenyldiacetylene	94.20	80.72
4,4'dihydroxydiphenyl-2,2-propane	30.10	22.09
4,4'-dinitrodiphenyl ether	10.29	22.70
4,4'-diundecanoyloxydiphenyldiacetylene	61.89	74.82
4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	31.48	22.96
4[p-[bis(2-chloroethyl)amino]benzene]butanoic acid	29.18	42.86
4'4'-diaminodiphenyl ether	7.74	22.86
4-acetoxybenzoic acid	26.35	24.06
4-amino-6-(1,1-dimethylethyl)-3-(methylthio)1,2,4-triazin-5(4H)-one	18.00	21.45
4-aminoacetophenone	38.00	17.22
4-aminobenzoic acid	20.92	22.75
4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide	22.30	30.24
4-aminopyridine	20.07	13.85
4-benzoyl-1-naphthol	28.64	21.79
4-bromo-2,5-dichloroaniline	22.11	16.93
4-bromo-2,5-dichlorophenol	22.11	17.13
4-chloroazobenzene	27.20	16.83
4-chlorobenzoic acid	32.26	20.26
4-chlorobiphenyl	13.32	15.76
4-chlorobut-2-ynyl 3-chlorophenylcarbamate	26.91	25.45
4-chlorophenol	14.07	14.27
4-chlorophenoxyacetic acid	36.27	24.66
4-chlorophenyl 4-chlorobenzenesulfonate	23.63	20.37
4-chlorophenylbenzenesulfonate	21.44	19.35
4-ethoxy-4'fluorodiphenyldiacetylene	33.90	23.58

4-ethoxy-4'-trifluoromethyldiphenyldiacetylene	32.73	28.45
4-ethoxybenzoic acid	29.40	26.04
4-ethoxyisonitrosoacetanilide	7.60	35.59
4-ethoxyphenylacetic acid	23.00	25.89
4-ethylbenzoic acid	14.06	20.64
4-ethynyl-1-[(4-ethynylphenyl)methoxy]benzene	21.20	26.09
4-fluorotoluene	9.35	10.35
4-heptanone	16.16	15.97
4-hexylresorcinol	19.04	30.16
4-hydroxy-3,5-diiodobenzonitrile	33.63	22.96
4-hydroxyazobenzene	32.99	19.51
4-hydroxybenzoic acid	30.90	22.94
4-hydroxyphenylacetic acid	28.40	22.79
4-hydroxyphenylpropionic acid	28.90	24.90
4-iodobenzoic acid	35.24	22.22
4-methoxybenzoic acid	28.40	23.09
4-methoxyphenol	18.30	17.10
4-methoxyphenylacetic acid	21.80	18.22
4-methoxyphenylbutyric acid	25.30	27.99
4-methoxyphenylpropionic acid	28.50	25.04
4-methyl-7-aminocoumarin	32.09	22.15
4-methyl-7-diethylaminocoumarin	17.88	25.54
4-methyl-7-dimethylaminocoumarin	23.92	24.34
4-methyl-7-hydroxycoumarin	29.14	22.34
4-methylcyclohex-1-ene	6.63	11.74
4-methylheptane	10.84	16.61
4-methylpent-1-ene	4.93	5.78
4-methylphenanthrene	14.09	17.39
4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline	28.05	35.95
4-methylthiazole	8.90	11.14
4-methylthio-3,5-xylyl methylcarbamate	30.36	26.32
4-n-butoxy-2',3',4'-trifluorodiphenylacetylene	36.00	28.23
4-n-butoxy-4'-fluorodiphenylacetylene	25.40	28.19
4-n-butoxy-4'-trifluoromethyldiphenyldiacetylene	25.37	28.89
4-n-butoxybenzoic acid	22.26	31.94
4-n-butyl-3',4'-difluorodiphenylacetylene	25.30	22.81
4-n-butyl-3',4'-difluorodiphenyldiacetylene	24.33	24.10
4-n-butyl-4'-fluorodiphenylacetylene	18.50	22.79
4-n-ethoxy-2',3',4'-trifluorodiphenylacetylene	32.20	22.33
4-n-ethoxy-2',4'-difluorodiphenylacetylene	27.00	22.31
4-n-ethoxy-4'-fluorodiphenylacetylene	22.80	22.29
4-n-ethyl-3',4'-difluorodiphenylacetylene	16.60	16.91
4-n-hexyl-3',4'-difluorodiphenylacetylene	24.30	30.00
4-n-hexylbenzoic acid	20.22	32.44
4-n-hexyloxy-2',3',4'-trifluorodiphenylacetylene	30.80	34.13
4-n-hexyloxy-2',4'-difluorodiphenylacetylene	34.10	34.11
4-n-hexyloxy-3',4'-difluorodiphenylacetylene	33.10	34.11
4-n-hexyloxy-4'-trifluoromethyldiphenyldiacetylene	33.98	34.79
4-nitro-4'-methylbenzylidene aniline	27.30	16.27
4-nitro-5-methylphenol	27.40	17.47
4-nitroaniline	21.09	16.48
4-nitrophthalic anhydride	17.14	20.06
4-nitrotoluene	16.81	13.76

4-n-octyloxy-N-(3,5-dimethoxybenzylidene)aniline	35.30	44.25
4-n-octyloxy-N-(3,5-dimethylbenzylidene)aniline	37.73	38.12
4-n-octyloxy-N-(4-methoxybenzylidene)aniline	42.29	40.39
4-n-pentoxy-2',3',4'-trifluorodiphenylacetylene	33.10	31.18
4-n-pentoxy-4'-fluorodiphenylacetylene	27.20	31.13
4-n-pentoxybenzoic acid	25.21	34.89
4-n-pentyl-3',4'-difluorodiphenylacetylene	22.10	25.76
4-n-pentyl-3',4'-difluorodiphenyldiacetylene	30.86	27.05
4-n-pentyl-4'-fluorodiphenylacetylene	25.60	25.74
4-n-pentylbenzoic acid	16.38	29.49
4-n-propoxy-2',3',4'-trifluorodiphenylacetylene	26.10	25.28
4-n-propoxy-2',4'-difluorodiphenylacetylene	25.20	25.26
4-n-propoxy-4'-fluorodiphenylacetylene	27.10	25.24
4-n-propoxybenzoic acid	28.12	28.99
4-n-propyl-3',4'-difluorodiphenylacetylene	20.20	19.86
4-n-propyl-3',4'difluorodiphenyldiacetylene	22.03	21.15
4-n-propyl-4'-fluorodiphenylacetylene	24.10	19.84
4-octadecynoic acid	57.94	47.21
4-oxaheptane	10.77	16.89
4-propoxy-4'-trifluoromethyldiphenyldiacetylene	18.81	25.94
4-propylbenzoic acid	28.07	23.59
4'-propylbiphenyl-4-carbonitrile	22.70	23.22
4-tert-butylbenzoic acid	17.91	22.50
4-tert-butylphenol	14.52	16.51
4-trans-(3-fluoro-4-cyanophenyl)cyclohexyl (E)-but-2-enoate	21.10	31.68
4-trans-(4-bromophenyl)cyclohexyl (E)-2-butenoate	28.40	29.54
4-trans-(4-chlorophenyl)cyclohexyl (E)-2-butenoate	30.20	28.55
4-trans-(4-fluorophenyl)cyclohexyl (E)-2-butenoate	25.10	27.55
4-trans-(4-fluorophenylethyl)cyclohexyl (E)-butenoate	25.00	32.59
4-trans-(trifluoromethoxyphenyl)cyclohexyl (E)-but-2-enoate	21.60	32.27
4-trans-cyanocyclohexyl (E) 2-butenoate	24.40	26.53
5'-(trifluoromethanesulphonamide)acet-2',4-xylidide	37.66	31.54
5,5-bis(3,3-dimethylbutyl)2,2,8,8-tetramethylnonane	48.53	50.68
5,5-dimethylperhydro-1,3-oxazine-2-one	28.50	30.13
5,6,7,8-tetrahydroquinoline	9.08	16.83
5,6-dibutyl-5,6-bis(4-tert-butylphenyl)decane	43.10	63.99
5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid	37.67	28.79
5-amino-4-chloro-2-phenyl-3(2H)-pyridazinone	26.75	29.27
5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione	22.02	25.11
5-butyl-2-ethylamino-6-methylpyrimidin-4-ol	20.32	33.28
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	12.51	23.45
5-isopropyl-m-tolyl methylcarbamate	23.04	23.86
5-methyl N-(methylcarbamoyloxy)thioacetimidate	21.73	26.69
5-methyl-1,2,4-triazolo[3,4-b]benzothiazole	24.07	17.17
5-methylnonane	16.65	22.51
5-methyltetrazole	16.00	19.21
5-methylthiazole	7.65	11.14
5-nonanone	26.22	21.86
5-octadecynoic acid	54.41	47.21
6-(4-biphenyl)-1-hexene	15.10	23.00
6,8,9-trimethyladenine	23.10	24.17
6,9-dimethyl-8-butyladenine	36.00	30.68
6-deoxy-6-fluoro-D-glucopyranose	27.20	29.50

6-deoxy-D-glucopyranose	22.70	26.28
6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one	29.92	22.16
6-octadecynoic acid	54.92	47.21
7,8-benzoquinoline	14.10	17.40
7-octadecynoic acid	53.61	47.21
8-(4-biphenyl)-1-octene	21.00	28.90
8-[4-(4'-n-butylbiphenyl)]-1-octene	12.40	36.21
8-octadecynoic acid	55.30	47.21
9-fluorenone	18.12	18.34
9-heptadecanone	66.68	45.46
9H-pyrido[3,4-b]indole	25.50	22.50
9-methylfluorene	16.32	11.29
9-octadecynoic acid	54.87	47.21
a-(trifluoromethoxy)-a,a-difluoromethyl acetate	8.51	15.73
a,a'-dibromo-m-xylene	23.69	18.17
a,a'-dibromo-o-xylene	26.78	18.17
a,a'-dichloro-m-xylene	19.51	16.53
a,a'-dichloro-o-xylene	21.26	16.53
a,a'-dichloro-p-xylene	23.97	16.53
a-alanyl-a-alanine (DL)	33.20	33.08
acenaphthene	21.46	14.90
acenaphthylene	15.35	13.31
acetaldehyde	5.46	8.79
acetamide	15.60	16.17
acetanilide	21.67	21.46
acetone	5.72	8.83
acetonitile	9.06	9.33
acetylacetone enol	14.50	12.29
acetylene	7.18	8.89
a-chloroacetic acid	14.11	15.86
a-chloroacetic acid	16.30	15.86
acridine	18.58	17.40
acrylamide	15.33	16.86
acrylic acid	11.16	16.12
acrylonitrile	7.42	10.55
a-D-glucopyranose (a-D-glucose)	34.30	32.68
a-D-glucose	31.42	32.68
adipic acid	34.85	29.91
alanylglycine (with decomp)	56.60	32.74
allobarbitiol	32.31	26.63
a-methylacrylic acid	8.06	15.09
a-methylstyrene	11.92	10.03
a-naphthol	23.01	16.77
a-naphthyl acetate	20.21	22.61
androstanolone	27.06	22.09
aniline	10.54	13.05
anisaldazine	29.75	28.63
anthracene	29.37	16.59
anthraquinone	32.57	23.27
azelaic acid	32.67	38.76
azoxybenzene	17.93	18.89
azulene	17.53	13.06
b(4-chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	24.47	32.88

b-alanyl-b-alanine	58.30	33.08
barbital	24.98	30.59
benzaldehyde	9.33	12.97
benzamide	18.49	19.98
benzanilide	29.61	24.76
benzene	9.87	9.53
benzene-hexa-n-hexanoate	74.70	95.28
benzidine	19.10	21.75
benzil	23.74	21.02
benzimidazole	19.25	18.97
benzo[c]cinnoline	20.92	16.24
benzofluoranthene	18.47	17.44
benzoic acid	17.99	19.24
benzoic anhydride	17.15	15.24
benzonitrile	10.98	13.67
benzophenone	18.37	14.55
benzothiazole	12.80	13.88
benzothiophene	11.84	13.08
benzotrichloride	13.95	14.43
benzotrifluoride	13.77	8.97
benzoxazole	16.80	12.37
benzyl alcohol	8.79	14.39
benzyl benzoate	20.44	22.32
benzylbromide	13.20	13.85
benzyliodide	13.20	15.77
benzylmethylsulfone	25.52	20.48
biphenyl	18.66	14.73
bis(2-cyanoethyl)-N-nitroamine	44.99	30.38
bis-(4-aminophenyl)methane	9.23	23.29
bis(4-chlorophenyl)acetic acid	31.66	25.84
bis-[3,5-di-tert-butyl-4-hydroxybenzyl]sulfide	43.10	41.65
bis-hydroxyethylpiperazine	25.90	32.22
bromobenzene	10.70	11.55
bromocyclohexane	10.79	16.24
bromomethane	5.98	6.43
bromotrichloromethane	7.69	9.92
butanal	11.09	12.35
butane	7.23	9.42
butanoic acid	11.07	16.72
butyl 4-aminobenzoate	20.46	27.26
butyl 9-hydroxy-9H-fluorene-9-carboxylate	25.56	25.70
butyl acrylate	17.31	20.63
butyl alcohol	9.28	15.82
butyl butanoate	14.93	21.45
butyl ethyl sulfide	12.39	18.13
butyl octadecanoate	39.70	62.74
caffeine	24.37	26.32
carbazole	26.94	21.69
carbon tetrabromide	10.70	12.38
carbon tetrachloride	7.79	9.10
carbon tetrafluoride	2.42	1.82
chlorobenzene	9.55	10.56
chlorocyclohexane	10.47	15.42

chlorocyclopentane	8.75	13.09
chlorodifluoromethane	4.19	2.81
chloroethane	4.45	8.56
chloroethyl methacrylate	17.00	18.74
chloropentafluorobenzene	14.29	10.67
chlorotrifluoroethylene	5.55	5.66
cholesterol*	30.91	29.96
chroman	16.26	18.02
chromone	17.31	18.49
chrysene	29.37	20.12
cinnamic acid	22.63	24.57
cinnamic anhydride	32.77	25.91
cinnamyl alcohol	15.73	16.39
cis,cis-1,3,5-tri-tert-butylcyclohexane	26.78	26.16
cis,trans-1,3,5-tri-tert-butylcyclohexane	17.99	26.16
cis-1,2-cyclohexanediol	23.83	19.46
cis-1,2-dimethylcyclohexane	12.33	12.67
cis-1,2-dimethylcyclopentane	11.97	10.34
cis-1,3-dimethylcyclohexane	10.82	12.67
cis-1,4-dimethylcyclohexane	9.29	12.67
cis-1,4-di-tert-butylcyclohexane	8.79	21.63
cis-2-butene	7.31	5.14
cis-2-hexene	8.88	8.71
cis-2-pentene	7.11	5.76
cis-3-chloro-2-butenoic acid	13.81	18.64
cis-6-octadecenoic acid	47.50	49.06
cis-9-octadecenoic acid	39.60	49.06
cis-crotonic acid	12.57	17.39
coronene	19.20	21.18
cortisone	36.86	29.89
cortisone acetate	38.43	31.96
coumarin	19.14	17.92
cyanamide	8.76	9.80
cyanoacetamide	22.90	21.11
cyanocyclohexane	13.48	17.66
cyanogen	8.11	10.86
cyclobutane	8.23	9.32
cycloheptane	12.62	16.31
cycloheptanol	8.00	19.05
cycloheptatriene	3.51	11.54
cycloheptene	9.14	14.72
cyclohexane	12.81	13.98
cyclohexanethiol	10.00	13.41
cyclohexanol	11.67	16.72
cyclohexanone	10.95	15.93
cyclohexanone oxime	9.69	17.71
cyclohexene	8.46	12.39
cyclohexylbenzene	15.30	18.65
cycloocta-1,5-diene	9.83	15.46
cyclooctane	14.08	18.64
cyclooctanol	4.45	21.38
cyclooctatetraene	11.25	12.28
cyclooctene	15.16	17.05

cyclopentadiene	8.01	8.47
cyclopentane	8.26	11.65
cyclopentanethiol	7.83	11.08
cyclopentanol	6.25	14.39
cyclopentene	4.12	10.06
cyclopentyl methyl sulfide	10.10	13.81
cyclopentylamine	8.79	16.40
cyclopropane	5.44	6.99
cyclopropylamine	13.18	11.74
D mannitol	56.10	35.07
D sorbitol	30.20	35.07
decachlorobiphenyl	39.34	25.02
decacyclene	25.40	31.77
decanal	30.60	30.05
decanoic acid	27.82	34.41
decyl methacrylate	30.55	33.77
deoxycorticosterone	27.98	25.54
deoxycorticosterone acetate	29.66	26.07
dexamethasone	42.02	27.97
diaminoethane	23.07	14.19
dibenzo[c,e][1,2]dithiin	19.30	18.22
dibenzodioxin	23.20	16.78
dibenzofuran	18.60	15.10
dibenzothiophene	21.58	16.61
dibromodichloromethane	8.48	10.74
dibromodifluoroethylene	7.04	8.64
dichloroacetic acid	12.34	17.27
dichloromethane	6.16	9.63
dicyanomethane	10.80	14.27
diethyl disulfide	9.40	15.04
diethyl ether	7.19	10.99
diethyl o-phthalate	17.99	26.16
diethyl sulfide	11.92	12.23
diethyl terephthalate	24.69	26.16
diethylstilbestrol	31.63	27.58
difluoromethane	4.36	6.00
dihydroxyethane	9.96	16.32
diiodomethane	12.05	15.10
diisopropyl ketone	11.20	10.74
diisopropyl sulfide	10.42	8.92
dimethoxymethane	8.33	9.61
dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	25.00	24.87
dimethyl amine	5.37	8.23
dimethyl ether	4.94	5.09
dimethyl fumarate	35.15	20.96
dimethyl maleate	14.64	20.96
dimethyl oxalate	21.07	29.53
dimethyl sulfide	7.98	6.33
dimethyl sulfoxide	14.37	12.91
dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	30.23	24.37
dimethylaminoethyl methacrylate	16.85	19.67
dimethyldisulfide	9.19	8.32
dimethylsulfone	18.28	14.54

di-n-butyl succinate	29.21	33.48
di-n-butyl sulfide	18.59	24.03
diphenyl ether	17.21	15.83
diphenyl sulfone	21.78	19.41
diphenylacetic acid	31.25	23.78
diphenylacetylene	20.50	15.46
diphenylamine	17.86	21.06
diphenylcarbinol	23.00	19.03
diphenylmethane	18.58	16.26
diphenylsulfide	13.98	15.25
dipropyl disulfide	13.81	20.12
dipropyl sulfide	12.13	18.13
DL 3,6-dimethyl-1,4-dioxane-2,5-dione	24.70	17.66
DL lactic acid	11.34	17.31
d-limonene	11.38	14.84
dodecane	36.82	33.01
dodecanedioic acid	50.57	47.60
dodecanoic acid	36.65	40.31
dodecanol	40.17	39.41
dotriacontane	117.94	91.99
dulcitol	65.10	35.07
d-valerolactone	11.29	16.47
E-3-chloro-2-butenoic acid	13.81	19.94
e-caprolactam	16.10	25.70
e-caprolactone	13.82	18.80
eicosanoic acid	69.20	63.90
estrone	48.03	22.76
ethane	2.79	3.52
ethanethioamide	18.36	19.29
ethanoic acid	11.72	13.15
ethanol	9.12	9.92
ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	32.75	41.39
ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	23.48	26.20
ethyl 4-aminobenzoate	23.56	21.36
ethyl acetate	10.48	11.99
ethyl carbamate	15.23	20.13
ethyl cyanoacetate	11.78	16.93
ethyl docosanoate	28.74	68.64
ethyl eicosanoate	23.36	62.74
ethyl hexaconsanate	40.27	80.43
ethyl hexadecanoate	15.09	50.94
ethyl mercaptan	4.97	6.56
ethyl methyl sulfide	9.76	9.28
ethyl N-benzoyl-n-(3,4-dichlorophenyl)-dl-alaninate	27.06	27.59
ethyl nitrate	8.53	8.72
ethyl phenyl carbamate	16.27	22.08
ethyl propyl ether	8.39	13.94
ethyl propyl sulfide	10.58	15.18
ethyl tetracosanate	34.14	86.33
ethyl triacontanoate	52.27	92.23
ethyl(1,1-dimethylpropyl)malononitrile	19.25	22.54
ethylbenzene	9.16	10.94
ethylcyclohexane	8.33	16.28

ethylcyclopentane	6.86	13.95
ethylene	3.35	2.60
ethylene carbonate	13.30	16.44
ethylene oxalate	13.40	18.57
ethylene oxide	5.17	8.98
ethylmethylsulfone	11.30	15.16
fluorene	19.58	15.51
fluorobenzene	11.31	9.56
fluorotrichloromethane	6.90	7.28
furan	6.37	8.04
furfural	14.37	12.33
furfuryl alcohol	13.10	12.90
glutaric acid	23.36	26.96
glyceryl triacetate	25.80	27.26
glyceryl trilaurate	123.51	108.73
glyceryl trimyristate	152.20	126.43
glyceryl tripalmitate	179.37	144.12
glyceryl tristearate	203.26	161.82
heptadecanoic acid	58.77	55.05
heptanal	22.89	21.20
heptane	14.04	18.27
heptanoic acid	17.85	25.56
hexachlorobenzene	23.85	15.71
hexachlorocyclopropane	18.60	14.27
hexachloroethane	24.36	16.21
hexacontane	186.80	174.56
hexadecane	53.35	44.81
hexadecanoic acid	54.81	52.10
hexafluoroacetone	8.38	6.13
hexafluorobenzene	11.59	9.67
hexafluoroethane	8.90	5.30
hexamethylbenzene	22.38	14.29
hexanal	15.39	18.25
hexanamide	25.10	25.63
hexatriacontane	129.29	103.79
hexyl ethanoate	19.83	23.78
hexyl N-phenylcarbamate	32.76	33.88
hydrazobenzene (1,2-diphenylhydrazine)	17.65	26.09
hydrocinnamic acid	17.68	21.19
hydrocortisone	35.77	30.69
hydrocortisone-21-acetate	37.02	32.75
imidazole	12.80	15.44
indene	10.20	12.11
iodobenzene	9.75	12.52
iodomethane	9.12	8.35
isobutane	4.56	4.81
isobutene	5.92	6.18
isobutyl alcohol	6.32	11.21
isobutyl mercaptan	4.98	7.85
isochroman	16.75	18.02
isonicotinic acid	32.14	20.04
isopropyl 4,4'-dibromobenzilate	24.55	26.52
isopropyl ether	12.05	7.68

isopropyl methyl ketone	9.34	9.79
isopropyl methyl sulfide	9.36	7.63
isopropyl nitrate	10.10	10.50
isopropyl phenylcarbamate	19.37	22.62
isopropyl-3-chlorophenylcarbamate	17.75	23.65
isopropylbenzene	7.32	11.28
isoquinoline	13.54	13.87
L-carvone	11.55	16.78
levulinic acid	9.22	19.70
L-iditol	30.90	35.07
linoelaidic acid	47.70	40.97
maleic anhydride	12.26	12.99
malonamide	37.70	27.94
m-aminophenol	22.98	16.76
m-bromophenol	15.10	15.26
methacrylamide	15.00	15.84
methanethiol	6.15	3.61
methanol	3.77	6.97
methoxybenzene	14.07	13.39
methyl 2-(2,4,5-trichlorophenoxy)acetate	30.46	22.61
methyl 2-(2,4,5-trichlorophenoxy)butyrate	28.87	25.90
methyl 2-(2,4,5-trichlorophenoxy)propionate	31.95	22.95
methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	27.08	28.22
methyl 2,4-dichlorophenoxyacetate	25.10	21.58
methyl 3,6-dichloro-2-methoxybenzoate	18.49	20.81
methyl 3-m-tolylcarbamoyloxyphenylcarbamate	39.62	39.23
methyl 4-(2,4-dichlorophenoxy)butyrate	32.64	27.48
methyl 4-amino-3,5,6-trichloro-2-picolinate	26.78	21.92
methyl 4-aminobenzoate	22.55	18.41
methyl 4-hydroxybenzoate	24.31	18.61
methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	26.31	26.69
methyl acetate	7.49	9.04
methyl acrylate	9.73	11.78
methyl a-D-mannopyranoside	44.70	30.85
methyl benzoate	13.90	14.90
methyl butyl sulfide	12.45	15.18
methyl carbamate	16.70	17.18
methyl chloride	6.42	5.61
methyl docosanoate	29.20	65.69
methyl isopropyl ether	5.85	6.38
methyl methacrylate	12.24	10.75
methyl myristate	50.21	42.09
methyl n-butyl ether	10.85	13.94
methyl n-decyl ether	31.71	31.63
methyl nitrate	8.24	9.21
methyl N-phenylcarbamate	14.56	21.33
methyl octadecanoate	19.23	53.89
methyl palmitate	68.16	47.99
methyl perfluorobutanoate	11.77	15.40
methyl p-N,N-dimethylaminobenzoate	26.07	17.64
methyl propyl ether	7.67	10.99
methyl propyl sulfide	9.91	12.23
methyl tert-butyl ether	7.60	9.80

methyl tert-butyl sulfide	8.41	11.05
methyl tetrachloroterephthalic acid ester	16.89	26.12
methyl-3,4-dichlorophenylcarbamate	23.19	23.38
methylamine	6.13	5.91
methylcyclobutane	5.76	8.67
methylcyclohexane	6.69	13.33
methylcyclopentane	6.93	11.00
methylenecyclobutane	5.86	8.50
methylhydrazine	10.42	10.72
methylphenylsulfide	14.85	12.94
methylphosphonyl chlorofluoride	11.85	12.54
methylphosphonyl dichloride	18.08	13.55
methylphosphonyl difluoride	11.88	10.46
m-hydroxytoluene	10.71	14.04
m-nitrobenzoic acid	19.33	22.67
m-nitrophenol	19.19	16.68
mono(2,2-dimethylhydrazide) butanedioic acid	36.97	33.25
m-phenylenediamine	15.40	16.56
m-terphenyl	22.59	19.92
m-toluic acid	15.73	20.03
m-toluidine	8.80	13.84
m-xylene	11.59	11.12
myo-inositol	47.90	30.43
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	25.19	28.04
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine	23.08	32.47
N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	29.13	26.70
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	32.04	22.67
N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea	27.48	29.91
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	16.35	30.14
N-(4-chlorophenyl)-2,2-dimethylpentanamide	23.31	30.86
N'-(4-chlorophenyl)-N-methoxy-N-methylurea	22.54	25.31
N-(cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl) benzenamine	22.51	30.25
N,N'-(2-hydroxyethyl)-1,4-diaminoanthraquinone	32.34	50.27
N,N-(2-hydroxyethyl)-4-(4-nitrophenyl)azoaniline	32.43	40.67
N,N-(2-hydroxyethyl)-4-phenylazoaniline	29.96	37.23
N,N-diethyl-2-(1-naphthyloxy)propionamide	24.57	30.52
N,N-dimethyl-1,3-propanediamine	12.38	17.77
N,N-dimethyl-2,2-diphenylacetamide	25.43	20.90
N,N-dimethyl-2,2-diphenylbenzeneacetamide	25.43	25.26
N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide	30.17	32.43
N,N-dimethyl-4-phenylazoaniline	23.08	18.54
N,N-dimethylaniline	12.75	12.28
N,N-dimethylformamide	8.95	11.43
N,N'-dimethylhydrazine	13.64	15.45
N,N-dimethylhydrazine	10.07	10.80
N,N'-dimethyl-N,N'dinitro-1,2-ethanediamine	60.32	25.63
N,N'-dimethyl-N,N'dinitro-1,6-hexanediamine	61.68	37.43
N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea	29.82	27.61
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea	33.87	26.77
N,N'-di-n-hexyladipamide	40.79	65.38
N,N'-dinitro-diaminomethane	35.85	26.77

N,N'-dinitroethanediamine	29.50	29.72
N,N'-di-n-propyladipamide	36.11	47.69
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	43.10	27.89
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-propanamide	23.85	40.61
N-[4-methyl-3-[[(trifluoromethyl)sulfonyl]amino]phenyl]acetamide	40.47	30.75
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea	29.48	27.95
N-acetyl-D-leucine amide	20.20	33.98
N-acetylglycine amide	25.60	29.40
N-acetylglycyl-L-prolinamide	32.60	39.81
N-acetyl-L-alanine amide	21.70	29.55
N-acetyl-L-isoleucinamide	41.80	33.98
N-acetyl-L-prolyl-glycinamide	32.20	39.81
N-acetyl-pyrazinamide	23.60	22.39
N-acetylsarcosinamide	27.40	23.53
N-allyl-N-phenylthiourea	27.61	28.44
naphthalene	19.10	13.06
naphthalene 1,8-disulfide	13.00	15.04
naphthalene 1,8-disulfide s-oxide	23.30	21.06
N-benzylaniline	16.76	22.40
N-butyl dodecanamide	39.00	52.15
n-butyl mercaptan	10.46	12.46
N-butyl tetradecanamide	45.00	58.04
n-butylbenzene	11.22	16.84
n-butylcyclohexane	14.14	22.17
n-butylcyclopentane	11.31	19.84
N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea	27.23	35.93
N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline	36.50	30.38
N-butylurea	23.77	28.18
n-decane	28.70	27.11
N-decyl hexadecanamide	68.00	81.64
n-decyl-a-cyanoacrylate	41.80	38.56
N-decylundecanamide	42.52	66.89
N-dimethylaminosuccinamic acid	36.97	34.31
n-docosane	77.30	62.50
n-dodecylcyclohexane	45.84	45.77
n-dononacontahectane	698.90	563.83
n-eicosane	67.80	56.60
neopentyl-4,4,4-trinitrobutyrate	22.59	30.07
n-ethyl-a-cyanoacrylate	12.86	14.96
N-ethylurea	14.39	22.28
n-hectane	333.00	292.52
n-heneicosane	63.18	59.55
n-heptacosane	87.59	77.25
n-heptadecane	51.13	47.76
N-heptylmyristamide	55.56	66.89
n-hexacosane	91.70	74.30
n-hexane	13.08	15.32
N-hexyl decanamide	37.00	52.15
N-hexyl hexadecanamide	57.00	69.84
N-hexyl tetradecanamide	50.00	63.94
nicotinic acid	27.48	20.04
N-isopropylcarbazole	18.75	20.00

N-isopropylurea	14.59	20.62
nitrobenzene	12.12	12.97
nitroethane	9.85	8.72
nitromethane	9.70	8.10
N-laurylnonanamide	67.08	66.89
N-methyl O-methyl O-2-chloro-4-tert-butylphenyl phosphoramidate	21.98	22.73
N-methyl-2,4,6,N-tetranitroaniline	25.86	27.26
N-methyl-2-chlorophenylcarbamic acid ester	21.81	22.36
N-methylacetamide	9.73	16.14
N-methylcarbazole	17.15	19.05
N-methyldiphenylacetamide	30.23	26.77
N-methyl-N-nitrobutanamine	37.56	20.48
N-methylpyrrole	7.82	11.99
N-methylurea	14.06	19.33
N-myristylheptanamide	54.76	66.89
N-nitro-bis(N,N-cyanomethyl) amine	38.66	24.49
N-nitro-N-methylaminomethane	37.66	11.63
n-nonacosane	95.81	83.15
n-octacosane	100.10	80.20
n-octane	20.74	21.22
n-octylbenzene	29.96	28.64
nonadecane	61.06	53.66
nonadecanoic acid	67.38	60.95
nonanal	29.60	27.10
nonane	21.76	24.17
nonanoic acid	26.28	31.46
nonyl acrylate	23.36	35.37
nonyl phenylcarbamate	28.07	44.92
N-palmitoyl-pyrazinamide	51.82	61.35
n-pentacontane	185.00	145.07
n-pentacosane	83.81	71.35
n-pentadecane	43.77	41.86
n-pentatriacontane	127.49	100.84
N-phenyl-N[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)	22.51	36.16
n-propylbenzene	9.27	13.89
n-propylcyclohexane	10.37	19.22
N-propylstearamide	66.06	66.89
N-propylurea	14.63	25.23
N-salicylidene-m-aminobenzoic acid	33.11	25.45
N-stearylpropanamide	57.87	66.89
N-tert-butylurea	33.23	24.05
n-tetracosane	86.19	68.40
n-tetratetracontane	145.50	127.38
n-tricosane	75.73	65.45
n-tridecane	36.50	35.96
n-undecane	29.37	30.06
N-vinylpyrrolidone	15.28	16.42
O-(2,4-dichlorophenyl) O-methyl-(1-methylethyl) phosphoramidothioate	29.33	24.38
O-(2-chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate	29.08	21.57
O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate	31.15	21.18
O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphonothioate	31.35	22.29
O,O,O',O'-tetramethyl O,O'-thiodi-p-phenylene bis(phosphorothioate)	33.03	30.39
O,O-diethyl O-4-nitrophenyl phosphorothioate	15.72	26.44

O,O-diethyl O-quinoxalin-2-yl phosphothioate	25.40	28.14
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl) phosphate	15.61	25.04
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	24.53	26.90
O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	30.61	35.10
O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	18.94	20.19
O,O-dimethyl O-(4-aminosulfonylphenyl)phosphorothioate	26.21	19.31
O,O-dimethyl O-4-nitrophenyl phosphorothioate	20.07	20.54
O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate	20.49	25.47
O,O-dimethyl S-phthalimidomethyl phosphorodithioate	26.96	26.03
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	25.92	21.00
O,S-dimethyl phosphoroamidothioate	13.34	18.18
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl O,O-diethyl phosphorothioate	27.32	35.91
o-aminophenol	34.00	16.38
octadecanamide	59.91	61.02
octadecane	61.50	50.71
octadecanoic acid	61.21	58.00
octadecanol	70.08	57.10
octafluoropropane	4.97	9.53
octafluorotetrahydrothiophene	21.98	11.26
octanal	25.86	24.15
octanoic acid	21.38	28.51
octyl methacrylate	24.09	29.09
O-ethyl O-(4-nitrophenyl)phenylphosphonothioate	25.05	24.60
o-hydroxyacetanilide	21.25	24.34
o-hydroxybiphenyl	15.91	18.44
o-hydroxytoluene	15.82	14.04
o-nitrobenzoic acid	27.99	22.03
o-nitrophenol	17.45	15.38
o-phenylenediamine	23.10	13.97
o-phenylenepyrene	21.51	17.80
o-terphenyl	17.20	19.92
o-toluic acid	20.17	20.03
o-toluidine	9.31	13.84
o-xylene	13.60	11.12
p,p'-dichlorobenzophenone	30.12	16.61
p-a-cumylphenol	21.68	18.38
p-aminobenzene sulphonamide	25.65	15.26
p-aminophenol	26.00	16.76
p-benzoquinone	18.45	16.21
p-bromotoluene	15.15	12.34
p-chlorobenzyl p-chlorophenyl sulfide	32.22	22.42
p-chlorotoluene	13.55	11.36
p-dioxanone	16.14	18.46
pentabromophenol	31.98	22.94
pentachloroaniline	18.70	17.81
pentachlorobenzene	20.60	14.68
pentachloronitrobenzene	18.41	18.11
pentachlorophenol	17.15	18.01
pentadecanoic acid	49.64	49.16
pentaerythritol	58.60	33.83
pentaerythritol tetrafluoride	16.74	21.12
pentaerythrityl tetrabromide	27.97	31.67

pentafluoroaniline	18.21	12.78
pentafluorobenzene	10.88	9.64
pentafluorochloroethane	7.57	7.12
pentafluoroethane	2.25	5.23
pentafluoronitrobenzene	11.81	13.08
pentafluorophenol	17.57	12.97
pentamethylbenzene	12.91	13.49
pentane	8.40	12.37
pentanoic acid	14.16	19.67
pentyl 4-aminobenzoate	23.93	30.21
perfluorotoluene	11.49	9.08
perylene	31.88	20.48
p-ethoxyacetanilide	31.25	28.27
phenanthrene	16.68	16.59
phenanthridine	22.85	17.40
phenazine	20.92	18.20
phenol	11.51	13.24
phenolphthalein	51.05	33.52
phenoxathiin	20.27	18.29
phenyl glycidyl ether	17.32	21.14
phenyl vinyl sulfone	11.72	15.27
phenylacetic acid	14.49	19.08
phenylacetylene	9.46	12.17
phenylaminoethyl methacrylate	25.47	28.11
phenylhydrazine	16.43	16.04
phenyl-o-tolylmethane	19.24	17.05
phenylurea	23.68	24.66
phthalazine	13.32	12.71
phthalic anhydride	23.09	16.63
p-hydroxyacetanilide	26.02	25.17
p-hydroxytoluene	12.72	14.04
picene	35.19	23.65
picolinic acid	30.00	20.04
picric acid	17.10	20.96
pimilic acid	27.62	32.86
p-iodotoluene	14.96	13.31
piperidine	14.85	15.03
pivaldehyde	10.49	11.26
p-methacryloyloxybenzoic acid	34.00	25.78
p-methoxyacetanilide	27.82	25.32
p-n-hexyloxybenzylideneaniline	31.75	30.64
p-nitrobenzoic acid	36.90	22.67
p-nitrophenol	18.25	16.68
p-phenylazoaniline	21.70	19.31
p-phenylenediamine	21.70	16.56
p-quaterphenyl	38.84	25.11
prednisolone	38.86	29.10
pregnenolone acetate	27.43	24.39
progesterone	26.92	21.47
propanal	8.59	9.40
propane	3.52	6.47
propene	2.93	3.87
propionic acid	10.66	13.77

propionitrile	6.78	9.95
propyl 4-aminobenzoate	20.54	24.31
propyl 4-hydroxybenzoate	27.99	24.50
propyl N-phenyl carbamate	21.08	27.22
propylcyclopentane	10.04	16.89
propylene carbonate	9.62	15.79
propylene oxide	6.57	8.33
p-terphenyl	37.46	19.92
p-toluic acid	22.72	20.03
p-toluidine	17.89	13.84
p-xylene	17.11	11.12
pyrazine	12.95	11.14
pyrazole	14.20	16.72
pyrene	18.38	16.95
pyridine	8.28	10.34
pyromellitic dianhydride 1,2,5,6-benzenetetracarboxylic dianhydride	15.82	23.72
pyrrole	7.91	14.63
pyrrolidine	9.12	12.70
quinazoline	16.95	14.67
quinoline	10.73	13.87
quinoxaline	11.80	14.67
S-(+)-4-isobutyl-a-methylphenyl acetic acid	18.70	22.58
S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate	25.22	30.64
S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethyl phoshorodithioate	27.76	24.74
S-2,3,3-trichloroallyl diisopropylthiocarbamate	27.11	21.24
S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl- O,O-dimethyl phosphorodithioate	28.54	26.22
sebacic acid	40.80	41.71
spiropentane	6.43	7.04
ß,ß-binaphthyl	38.90	21.79
ß-chloroacetic acid	12.09	15.86
ß-chloroacetic acid	13.93	15.86
ß-naphthol	18.79	16.77
ß-naphthyl acetate	20.05	22.61
ß-propiolactone	9.41	11.81
ß-thiolactic acid	16.97	14.00
styrene	10.96	11.05
suberic acid	28.82	35.81
succinic acid	32.95	24.01
succinimide	17.00	14.66
succinonitrile	12.51	16.38
terephthalyl dichloride	23.44	15.54
tert-butyl alcohol	8.02	10.72
tert-butyl amine	7.29	10.01
tert-butyl bromide	10.07	11.14
tert-butyl chloride	11.17	10.33
tert-butyl mercaptan	12.31	8.32
tert-butylbenzene	8.41	12.80
tert-butylmethylsulfone	24.69	17.02
testosterone	29.38	21.04
testosterone acetate	27.88	23.16

testosterone formate	26.36	20.09
testosterone propionate	25.64	23.78
testosterone valerate	24.57	29.68
tetra(methylthia)methane	19.13	19.48
tetrachloroethene	11.86	8.68
tetrachloro-o-xylene	21.46	15.23
tetrachloro-p-xylene	22.59	15.23
tetracontane	147.46	115.58
tetracyanoethylene	24.92	18.97
tetradecane	45.07	38.91
tetradecanoic acid	45.10	46.21
tetrafluoroethylene	7.71	4.65
tetrahydrofuran	8.54	13.64
tetramethylsuccinonitrile	30.34	20.09
tetramethylurea	13.40	13.88
tetramethysuccinic acid	22.75	27.72
tetratriacontane	109.24	97.89
tetrazole	17.70	18.41
theophylline	28.20	28.97
thiacyclobutane	8.91	13.78
thiacyclohexane	13.50	18.44
thiacyclopentane	7.35	16.11
thianthrene	27.55	19.80
thiazole	9.58	10.35
thiophene	6.69	9.55
thiophenol	11.48	11.43
thiourea	12.55	20.01
thioxanthene 50-195	26.10	18.70
thioxanthone	35.50	21.53
thymine	17.51	21.39
thymol	22.01	15.78
toluene	6.61	10.33
tolyl vinyl sulfone	10.88	16.06
trans,cis-2,6-octadiene-1,8-dioic acid	22.78	32.49
trans,trans-2,6-octadiene-1,8-dioic acid	41.39	32.49
trans-1-(4-heptanoylphenyl)-4-heptylcyclohexane	24.20	52.28
trans-1,2-cyclohexanediol	18.51	19.46
trans-1,2-dimethylcyclohexane	10.50	12.67
trans-1,3-dimethylcyclohexane	9.87	12.67
trans-1,3-dimethylcyclopentane	7.41	10.34
trans-1,3-pentadiene	7.14	9.21
trans-1,4-dimethylcyclohexane	12.34	12.67
trans-1,4-di-tert-butylcyclohexane	17.15	22.10
trans-10-octadecenoic acid	58.52	49.06
trans-11-octadecenoic acid	58.52	49.06
trans-12-octadecenoic acid	56.71	49.06
trans-13-octadecenoic acid	55.62	49.06
trans-14-octadecenoic acid	57.06	49.06
trans-15-octadecenoic acid	58.98	49.06
trans-1-heptyl-4-(4-nonanoylphenyl)cyclohexane	32.12	58.17
trans-2-butene	9.76	5.14
trans-2-pentene	8.35	5.76
trans-3-octadecenoic acid	57.15	49.91

trans-4-octadecenoic acid	55.88	49.06
trans-5-octadecenoic acid	45.11	49.06
trans-6-octadecenoic acid	60.15	49.06
trans-9-octadecenoic acid (elaidic acid)	61.55	49.06
trans-azobenzene	22.53	15.80
triacontane	106.32	86.09
triamcinolone	42.56	33.39
triatriacontane	105.02	94.94
tribromomethane	11.09	8.90
trichloroacetic acid	5.88	17.25
trichloroethylene	8.45	7.15
trichloromethane	8.80	6.45
tridecandioic acid	45.30	50.55
tridecanoic acid	42.69	43.26
tridecanol	45.41	42.36
trifluoroacetonitrile	4.97	7.98
trifluoromethane	4.06	0.99
trifluoromethanethiol	4.93	4.50
trifluoromethyl (2-hydroxy-1-propenyl)ketone	8.45	15.74
trimellitic anhydride(1,2,4-benzenetricarboxylic acid)	11.90	26.33
trimethylamine	6.54	6.54
trimethylhydrazine	9.49	12.61
trinitroglycerine	21.87	27.76
triphenyl phosphate	29.61	25.90
triphenylamine	24.89	12.59
triphenylchloromethane	27.90	22.08
triphenylene	24.74	20.12
triphenylmethane	21.97	20.96
triphenylphosphine oxide	24.22	17.66
tri-tert-butylmethanol	12.73	24.86
undecanedioic acid	39.65	44.66
undecanoic acid	34.45	37.36
undecanolactone	15.97	30.57
urea	12.93	18.06
vinyl acetate	8.46	7.91
vinyl chloride	4.92	4.11
xanthene	19.20	17.19
xanthone	26.12	20.03
Z-3-chloro-2-butenoic acid	20.71	18.64
z-enantholactam	13.78	28.03

APPENDIX C. Rotational symmetry number (σ), Flexibility count (Φ), experimental entropy of melting and predicted entropy of melting (ΔS_m) for 1663 organic compounds.

Name			ΔS_m (J/K.mol)	
	σ	Φ	exp	pred
(+)2-butanol	1	1.0	33.8	57.4
(+)a-(3-benzoylphenyl)propionic acid	1	1.0	76.8	57.4
(2,4,5-trichlorophenoxy)acetic acid	1	2.0	88.1	64.8
(2,4-dichlorophenoxy)acetic acid	1	2.0	85.6	64.8
(4-chloro-2-methylphenoxy)acetic acid	1	2.0	76.3	64.8
(4-chloro-o-tolyloxy)acetic acid	1	2.0	76.3	64.8
(d) 1,2-dibromoacenaphthene	2	0.0	63.4	44.3
(d) 1,2-dichloroacenaphthene	2	0.0	56.9	44.3
(d) 1,2-diphenyl-1,2-dihydroxyethane	1	2.0	81.6	64.8
(d) 2-(1-naphthoxy)propionamide	1	2.0	80.1	64.8
(D) 2-(2-chloro-3-methylphenoxy)propionic acid	1	2.0	61.7	64.8
(d) 2-(m-chlorophenoxy)propanoic acid	1	2.0	80.8	64.8
(d) 2-(o-chlorophenoxy)propanoic acid	1	2.0	72.6	64.8
(d) 2-(p-bromophenoxy)propanoic acid	1	2.0	72.7	64.8
(d) 2-(p-methoxyphenyl)propiophenone	1	2.0	66.7	64.8
(d) 2-(p-nitrophenoxy)propanoic acid	1	2.0	57.8	64.8
(d) 2,3-dibromo-1,4-butanediol	1	3.0	87.3	72.1
(d) 2-phenoxypropionic acid	1	2.0	62.9	64.8
(d) 3-(m-bromophenyl)-3-hydroxypropanoic acid	1	2.0	68.1	64.8
(d) 3-(m-chlorophenyl)-3-hydroxypropanoic acid	1	2.0	76.2	64.8
(d) 3-(m-fluorophenyl)-3-hydroxypropanoic acid	1	2.0	78.0	64.8
(d) 3-(o-fluorophenyl)-3-hydroxypropanoic acid	1	2.0	64.9	64.8
(d) 3-(p-bromophenyl)-3-hydroxypropanoic acid	1	2.0	89.3	64.8
(d) 3-(p-chlorophenyl)-3-hydroxypropanoic acid	1	2.0	72.8	64.8
(d) 3-(p-fluorophenyl)-3-hydroxypropanoic acid	1	2.0	81.3	64.8
(d) 3-hydroxy-3-phenylbutyric acid	1	2.0	63.3	64.8
(d) 3-hydroxy-3-phenylvaleric acid	1	3.0	81.7	72.1
(d) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid	1	2.0	92.2	64.8
(d) 3-phenyl-3-hydroxypropanoic acid	1	2.0	83.5	64.8
(d) dimethyl diacetyltartrate	1	7.0	77.7	101.7
(d) dimethyl tartrate	1	4.0	53.9	79.5
(d) malic acid	1	2.0	61.2	64.8
(d) mandelic acid	1	1.0	64.9	57.4
(d) methylenebisthiopropionic acid	1	5.0	63.6	86.9
(d) m-fluoromandelic acid	1	1.0	61.6	57.4
(d) o-chloromandelic acid	1	1.0	62.9	57.4
(d) o-fluoromandelic acid	1	1.0	57.6	57.4
(d) p-chloromandelic acid	1	1.0	58.4	57.4
(d) p-fluoromandelic acid	1	1.0	71.7	57.4
(dl) 1,2-dibromoacenaphthene	2	0.0	63.2	44.3
(dl) 1,2-dichloroacenaphthene	2	0.0	60.5	44.3
(dl) 1,2-diphenyl-1,2-dihydroxyethane	1	2.0	79.8	64.8

(dl) 2-(1-naphthoxy)propionamide	1	2.0	84.6	64.8
(dl) 2-(2-chloro-3-methylphenoxy)propionic acid	1	2.0	78.0	64.8
(dl) 2-(m-chlorophenoxy)propanoic acid	1	2.0	85.6	64.8
(dl) 2-(o-chlorophenoxy)propanoic acid	1	2.0	83.0	64.8
(dl) 2-(p-bromophenoxy)propanoic acid	1	2.0	82.6	64.8
(dl) 2-(p-methoxyphenyl)propiophenone	1	2.0	74.7	64.8
(dl) 2-(p-nitrophenoxy)propanoic acid	1	2.0	78.3	64.8
(dl) 2,3-dibromo-1,4-butanediol	1	3.0	80.6	72.1
(dl) 2-phenoxypropionic acid	1	2.0	85.2	64.8
(dl) 3-(m-bromophenyl)-3-hydroxypropanoic acid	1	2.0	76.7	64.8
(dl) 3-(m-chlorophenyl)-3-hydroxypropanoic acid	1	2.0	70.1	64.8
(dl) 3-(m-fluorophenyl)-3-hydroxypropanoic acid	1	2.0	70.7	64.8
(dl) 3-(o-fluorophenyl)-3-hydroxypropanoic acid	1	2.0	79.5	64.8
(dl) 3-(p-bromophenyl)-3-hydroxypropanoic acid	1	2.0	77.8	64.8
(dl) 3-(p-chlorophenyl)-3-hydroxypropanoic acid	1	2.0	83.2	64.8
(dl) 3-(p-fluorophenyl)-3-hydroxypropanoic acid	1	2.0	76.3	64.8
(dl) 3-hydroxy-3-phenylbutyric acid	1	2.0	59.6	64.8
(dl) 3-hydroxy-3-phenylvaleric acid	1	3.0	89.2	72.1
(DL) 3-methylnonane	1	6.0	99.2	94.3
(dl) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid	1	2.0	91.5	64.8
(dl) 3-phenyl-3-hydroxypropanoic acid	1	2.0	81.2	64.8
(DL) 4-methylnonane	1	6.0	86.9	94.3
(dl) dimethyl diacetyltartrate	1	7.0	73.0	101.7
(dl) dimethyl tartrate	1	4.0	74.8	79.5
(dl) malic acid I	1	2.0	83.4	64.8
(dl) malic acid II	1	2.0	76.2	64.8
(dl) mandelic acid	1	1.0	65.1	57.4
(dl) menthol	1	3.0	34.0	72.1
(dl) methylenebisthiopropionic acid	1	5.0	91.7	86.9
(dl) m-fluoromandelic acid	1	1.0	66.7	57.4
(dl) o-chloromandelic acid	1	1.0	56.0	57.4
(dl) o-fluoromandelic acid	1	1.0	77.2	57.4
(dl) p-chloromandelic acid	1	1.0	69.0	57.4
(dl) p-fluoromandelic acid	1	1.0	72.7	57.4
(l) menthol	1	3.0	37.6	72.1
[(benzoylamino)oxy] acetic acid	1	3.5	75.5	75.8
1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	1	3.0	65.1	72.1
1-(methylamino)-9,10-anthracenedione	1	1.0	65.0	57.4
1-(o-chlorophenyl)thiourea	1	1.5	53.9	61.1
1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)	1	2.0	68.8	64.8
1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene	1	4.0	76.2	79.5
1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene)	1	4.0	70.4	79.5
1,1'-(2,2-dichloroethylidenebis(4-chlorobenzene)	1	2.0	71.5	64.8
1,1-(di-p-chlorophenyl)-2-nitropropane	1	3.0	60.4	72.1
1,1,1,3-tetrachloropropane	1	1.0	53.4	57.4
1,1,1-trichloro-3,3,3-trifluoropropane	1	0.0	60.5	50.0
1,1,1-trichloroethane	3	0.0	42.2	40.9
1,1,1-trifluoro-3,3-dichloropropane	1	1.0	56.7	57.4
1,1,1-trifluoro-3-chloropropane	1	1.0	54.6	57.4
1,1,1-trifluoroethane	3	0.0	38.2	40.9
1,1,1-trifluoro-n-[2-methyl-4-(phenylsulphonyl)phenyl] methane sulfonamide	1	2.0	76.0	64.8

1,1,1-trinitroethane	1	0.0	49.6	50.0
1,1,2,2-tetrachlorodifluoroethane	1	0.0	18.4	50.0
1,1,2,2-tetrachloroethane	1	1.0	42.1	57.4
1,1,2-tribromoethane	2	0.0	37.3	44.3
1,1,2-trichloroethane	1	1.0	48.0	57.4
1,1,2-trifluoro-1,2,2-trichloroethane	1	0.0	20.5	50.0
1,1,3,3-tetraethylurea	1	5.5	81.2	90.6
1,1,3-trimethylurea	1	1.5	41.5	61.1
1,10-decanediol	1	9.0	120.7	116.4
1,12-benzoperylene	2	0.0	31.3	44.3
1,1-bis(4-chlorophenyl)-2-nitrobutane	1	4.0	46.7	79.5
1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene	2	0.0	65.3	44.3
1,1-dichloroethane	1	0.0	44.7	50.0
1,1-dichloroethene	2	0.0	43.1	44.3
1,1-dicyclohexyldodecane	1	15.0	147.5	160.7
1,1-diethylurea	1	2.5	59.5	68.5
1,1-difluoro-1-chloroethane	1	0.0	18.9	50.0
1,1-dimethyl-3-phenylurea	1	2.0	56.3	64.8
1,1-dimethylcyclohexane	1	3.0	47.4	72.1
1,1-dimethylcyclopentane	1	2.0	49.5	64.8
1,1-dimethylurea	1	0.5	64.1	53.7
1,1-diphenyldodecane	1	11.0	148.1	131.2
1,2,3,4,5,6,7,8-octahydroanthracene	1	2.0	60.4	64.8
1,2,3,4,5-pentahydroxypentane (D-Arabitol)	1	4.0	102.5	79.5
1,2,3,4,5-pentahydroxypentane (Ribitol)	1	4.0	100.3	79.5
1,2,3,4,5-pentahydroxypentane (Xylitol)	1	4.0	102.3	79.5
1,2,3,4-tetracarbomethoxybenzene	1	4.0	99.8	79.5
1,2,3,4-tetracarbomethoxynaphthalene	1	4.0	84.7	79.5
1,2,3,4-tetrachlorobenzene	2	0.0	53.1	44.3
1,2,3,4-tetrafluorobenzene	2	0.0	46.8	44.3
1,2,3,4-tetrahydronaphthlene	1	1.0	52.4	57.4
1,2,3,4-tetrahydroquinoline	1	1.0	40.7	57.4
1,2,3,4-tetrahydroxybutane	1	3.0	107.0	72.1
1,2,3,4-tetramethylbenzene	2	0.0	42.3	44.3
1,2,3,5-tetracarbomethoxybenzene	1	4.0	83.8	79.5
1,2,3,5-tetrachlorobenzene	2	0.0	58.7	44.3
1,2,3,5-tetrafluorobenzene	1	0.0	47.0	50.0
1,2,3,5-tetramethylbenzene	2	0.0	52.0	44.3
1,2,3,6,7,8-hexahydropyrene	2	0.0	57.7	44.3
1,2,3-tribromopropane	1	2.0	82.2	64.8
1,2,3-tricarbomethoxybenzene	1	4.0	87.0	79.5
1,2,3-tricarbomethoxynaphthalene	1	3.0	65.3	72.1
1,2,3-trichlorobenzene	2	0.0	62.7	44.3
1,2,3-trihydroxybenzene	2	0.0	45.6	44.3
1,2,3-trihydroxypropane	1	2.0	62.4	64.8
1,2,3-trimethylbenzene	2	0.0	41.0	44.3
1,2,4,5,8,9-tribenzopyrene	2	0.0	47.4	44.3
1,2,4,5-tetrabromobenzene	4	0.0	62.3	38.5
1,2,4,5-tetracarbomethoxybenzene	1	4.0	85.7	79.5
1,2,4,5-tetracarbomethoxynaphthalene	1	4.0	83.1	79.5
1,2,4,5-tetrachloro-3-nitrobenzene	1	0.0	52.1	50.0
1,2,4,5-tetrachlorobenzene	4	0.0	57.2	38.5
1,2,4,5-tetrafluorobenzene	4	0.0	54.3	38.5

1,2,4,5-tetramethylbenzene	4	0.0	59.3	38.5
1,2,4-triazole	1	0.0	40.9	50.0
1,2,4-tricarbomethoxynaphthalene	1	3.0	81.5	72.1
1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene	1	0.0	68.9	50.0
1,2,4-trimethylbenzene	1	0.0	57.5	50.0
1,2,5,6-tetracarbomethoxynaphthalene	1	4.0	89.5	79.5
1,2,5-tricarbomethoxynaphthalene	1	3.0	70.2	72.1
1,2,6,7-tetracarbomethoxynaphthalene	1	4.0	84.0	79.5
1,2,6-tricarbomethoxynaphthalene	1	3.0	86.2	72.1
1,2,7,8-tetrahydroxyoctane	1	7.0	104.2	101.7
1,2,7-tricarbomethoxynaphthalene	1	3.0	84.5	72.1
1,2,8-tricarbomethoxynaphthalene	1	3.0	67.6	72.1
1,2:3,4-dibenzanthracene	2	0.0	46.6	44.3
1,2:3,4-dibenzopyrene	1	0.0	49.2	50.0
1,2:4,5-dibenzopyrene	1	0.0	58.6	50.0
1,2:5,6-dibenzanthracene	2	0.0	57.3	44.3
1,2-benzacenaphthene (fluoranthene)	1	0.0	48.9	50.0
1,2-benzanthracene	1	0.0	49.2	50.0
1,2-benzofluorene	1	0.0	48.0	50.0
1,2-benzopyrene	2	0.0	42.0	44.3
1,2-bromochlorobenzene	1	0.0	47.5	50.0
1,2-bromoiodobenzene	1	0.0	49.0	50.0
1,2-butadiene	20	0.0	50.8	25.2
1,2-chloronitrobenzene	1	0.0	61.9	50.0
1,2-diamino-2-methylpropane	1	1.0	73.8	57.4
1,2-diaminopropane	1	1.0	78.2	57.4
1,2-dibenzoylethane	1	2.0	94.6	64.8
1,2-dibromo-1,1-difluoroethane	1	1.0	40.2	57.4
1,2-dibromobenzene	2	0.0	45.9	44.3
1,2-dibromoethane	1	1.0	46.4	57.4
1,2-dibromotetrafluoroethane	1	1.0	43.2	57.4
1,2-dicarbomethoxybenzene	1	2.5	61.8	68.5
1,2-dicarbomethoxynaphthalene	1	2.0	77.1	64.8
1,2-dichlorobenzene	2	0.0	50.4	44.3
1,2-dichloroethane	1	1.0	37.2	57.4
1,2-dichloropropane	1	1.0	37.1	57.4
1,2-dichloro-tetrafluoroethane	1	0.0	39.0	50.0
1,2-dicyanobenzene	2	0.0	48.3	44.3
1,2-difluoro-2,2-dichloroethane	1	0.0	50.2	50.0
1,2-difluorobenzene	2	0.0	48.9	44.3
1,2-dihydro-6-neopentyl-2-oxonicotinic acid	1	1.0	41.2	57.4
1,2-dihydroxybenzene	2	0.0	58.4	44.3
1,2-diiodobenzene	2	0.0	47.2	44.3
1,2'-dinaphthylmethane	1	1.0	82.6	57.4
1,2-dinitrobenzene	2	0.0	57.7	44.3
1,2-diphenyl-2-(N-piperidinyl)-1-ethanone	1	4.5	97.2	83.2
1,2-diphenylethane	1	2.0	78.3	64.8
1,2-pentadiene	1	0.5	55.6	53.7
1,3,3-trinitroazetidine	1	1.0	80.7	57.4
1,3,5,5-tetranitro-1,3-diazacyclohexane	1	3.0	68.3	72.1
1,3,5,7-tetroxane	1	5.0	58.7	86.9
1,3,5-tri-a-naphthylbenzene	1	3.0	89.5	72.1
1,3,5-tricarbomethoxynaphthalene	1	3.0	64.3	72.1

1,3,5-trichloro-2,4,6-trifluorobenzene	6	0.0	59.2	35.1
1,3,5-trichlorobenzene	6	0.0	54.1	35.1
1,3,5-trimethylbenzene	6	0.0	41.6	35.1
1,3,5-trinitro-1,3,5-triazacyclohexane	1	3.0	78.8	72.1
1,3,5-trinitrobenzene	1	0.0	43.9	50.0
1,3,5-trinitroso-1,3,5-triazacyclohexane	1	3.0	58.5	72.1
1,3,5-trioxane	1	3.0	45.3	72.1
1,3,5-triphenylbenzene	1	1.0	74.9	57.4
1,3,6-trimethyluracil	1	0.0	55.1	50.0
1,3,7-tricarbomethoxynaphthalene	1	3.0	83.3	72.1
1,3,7-trichlorodibenzodioxin	1	0.0	73.0	50.0
1,3,8-tricarbomethoxynaphthalene	1	3.0	71.4	72.1
1,3-bromochlorobenzene	1	0.0	48.8	50.0
1,3-bromoiodobenzene	1	0.0	43.0	50.0
1,3-butadiene	2	0.0	48.6	44.3
1,3-cyclohexadiene	1	1.0	26.1	57.4
1,3-dibromobenzene	2	0.0	49.6	44.3
1,3-dibromopropane	1	2.0	61.4	64.8
1,3-dibutylurea	1	7.5	78.5	105.4
1,3-dicarbomethoxybenzene	1	2.5	74.2	68.5
1,3-dicarbomethoxynaphthalene	1	2.0	80.5	64.8
1,3-dichlorobenzene	2	0.0	50.9	44.3
1,3-dicyanopropane	1	2.0	51.6	64.8
1,3-diethylurea	1	3.5	37.4	75.8
1,3-difluorobenzene	2	0.0	46.1	44.3
1,3-dihydroxybenzene	2	0.0	52.5	44.3
1,3-diiodobenzene	2	0.0	51.8	44.3
1,3-dimethyluracil	1	0.0	36.7	50.0
1,3-dimethylurea	1	1.5	36.5	61.1
1,3-dinitro-1,3-diazacycloheptane	1	3.0	66.6	72.1
1,3-dinitro-1,3-diazacyclohexane	1	3.0	54.5	72.1
1,3-dinitro-1,3-diazacyclopentane	1	2.0	62.3	64.8
1,3-dinitro-5-nitroso-1,3,5-triazacyclohexane	1	3.0	58.2	72.1
1,3-dinitrobenzene	1	0.0	47.8	50.0
1,3-dioxolane	1	2.0	56.1	64.8
1,3-diphenylacetone	1	2.0	65.8	64.8
1,3-diphenylurea	1	2.0	67.6	64.8
1,3-dithiane	1	3.0	46.5	72.1
1,3-nitrochlorobenzene	1	0.0	61.0	50.0
1,4,5,8-tetracarbomethoxynaphthalene	1	4.0	75.6	79.5
1,4,5-tricarbomethoxynaphthalene	1	3.0	65.9	72.1
1,4,6-tricarbomethoxynaphthalene	1	3.0	73.8	72.1
1,4-[bis[(4-methylphenyl)amino]-9,10-anthracenedione	1	2.0	74.5	64.8
1,4-bis(diphenylphosphino)butane	1	10.0	111.6	123.8
1,4-bis(phenylglyoxaloyl)benzene	1	4.0	76.0	79.5
1,4-bis-[4-(4'-n-butylbiphenyl)]butane	1	10.0	81.3	123.8
1,4-bromochlorobenzene	2	0.0	55.5	44.3
1,4-bromoiodobenzene	2	0.0	52.7	44.3
1,4-cyclohexadiene	2	0.0	29.2	44.3
1,4-cyclohexanedione	1	2.0	49.3	64.8
1,4-diamino-2-methoxyanthraquinone	1	1.0	68.5	57.4
1,4-diaminoanthraquinone	2	0.0	50.0	44.3
1,4-dibromobenzene	4	0.0	55.7	38.5

1,4-dicarbomethoxybenzene	1	2.5	77.5	68.5
1,4-dicarbomethoxynaphthalene	1	2.0	60.0	64.8
1,4-dichloro-2,5-dimethoxybenzene	1	1.5	68.2	61.1
1,4-dichlorobenzene	4	0.0	55.7	38.5
1,4-dihydroxybenzene	4	0.0	59.5	38.5
1,4-dihydroxybutane	1	3.0	63.7	72.1
1,4-diiodobenzene	4	0.0	55.6	38.5
1,4-dimethylnaphthalene	2	0.0	37.9	44.3
1,4-dinitrobenzene	4	0.0	63.0	38.5
1,4-dioxane	1	3.0	53.5	72.1
1,4-dioxane-2,5-dione	1	0.0	47.4	50.0
1,4-di-tert-butylbenzene	1	0.0	65.8	50.0
1,4-dithiane	1	3.0	56.2	72.1
1,4-nitrochlorobenzene	2	0.0	33.4	44.3
1,4-pentadiene	1	1.0	49.4	57.4
1,5-cyclooctanedione	1	4.0	34.9	79.5
1,5-dicarbomethoxynaphthalene	1	2.0	67.3	64.8
1,5-dichloro-3-oxapentane	1	4.0	37.0	79.5
1,5-dimethyltetrazole	1	0.0	42.1	50.0
1,5-dinitro-3-nitroso-1,3,5-triazacycloheptane	1	4.0	70.2	79.5
1,5-pentanediol	1	4.0	63.4	79.5
1,6-bis-[4-(4'-ethylbiphenyl)]hexane	1	9.0	92.1	116.4
1,6-dicarbomethoxynaphthalene	1	2.0	59.4	64.8
1,6-hexanediol	1	5.0	79.6	86.9
1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane	1	9.0	91.1	116.4
1,7-dicarbomethoxynaphthalene	1	2.0	55.1	64.8
1,7-heptanediol	1	6.0	72.2	94.3
1,8-bis-(4-biphenyl)octane	1	8.0	134.9	109.1
1,8-bis-[4-(4'-ethylbiphenyl)]butane	1	6.0	101.3	94.3
1,8-bis-[4-(4'-ethylbiphenyl)]octane	1	10.0	122.0	123.8
1,8-bis-[4-(4'-n-butylbiphenyl)]octane	1	14.0	97.2	153.3
1,8-dimethylnaphthalene	2	0.0	46.9	44.3
1,8-octanediol	1	7.0	108.5	101.7
1,9-nonanediol	1	8.0	113.9	109.1
10H-phenothiazine	1	0.0	58.8	50.0
10-nonadecanone	1	16.0	202.0	168.1
10-octadecynoic acid	1	14.0	164.0	153.3
11-cyclohexyleicosane	1	19.0	180.4	190.3
11-heneicosanone	1	18.0	226.3	182.9
11-n-decylheneicosane	1	28.0	252.0	256.7
11-octadecynoic acid	1	14.0	174.9	153.3
11-phenyleicosane	1	18.0	220.1	182.9
12-octadecynoic acid	1	14.0	155.6	153.3
12-tricosanone	1	20.0	228.0	197.6
13-octadecynoic acid	1	14.0	172.4	153.3
14-octadecynoic acid	1	14.0	156.5	153.3
16-octadecynoic acid	1	14.0	173.2	153.3
17-octadecynoic acid	1	15.0	159.4	160.7
1-8-naphthalic anhydride	2	0.0	43.0	44.3
1a,2a,3ß,4a,5a,6ß-hexachlorocyclohexane	1	3.0	57.2	72.1
1-acetoxynaphthalene	1	1.0	63.3	57.4
1-acetyl-2-naphthol	1	0.0	63.3	50.0
1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione	1	1.0	67.2	57.4

1-aminoanthraquinone	1	0.0	54.9	50.0
1-aminopropane	1	1.0	58.2	57.4
1-benzoyl-2-naphthol	1	0.0	75.7	50.0
1-bromo-2-chloro-1,1,2-trifluoroethane	1	1.0	30.0	57.4
1-bromo-2-chloroethane	1	1.0	54.7	57.4
1-bromobutane	1	2.0	57.5	64.8
1-bromodocosane	1	21.0	218.0	205.0
1-bromoheptane	1	5.0	101.5	86.9
1-bromohexane	1	4.0	96.0	79.5
1-bromonaphthalene	1	0.0	55.9	50.0
1-bromononane	1	7.0	123.8	101.7
1-bromooctane	1	6.0	113.2	94.3
1-bromopentane	1	3.0	77.6	72.1
1-bromotricosane	1	29.0	310.2	264.1
1-bromoundecane	1	9.0	127.1	116.4
1-butene	1	0.5	43.8	53.7
1-butyne	1	0.0	40.9	50.0
1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl) benzene	1	2.0	66.8	64.8
1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl) benzene	1	0.0	68.2	50.0
1-chloro-2,2-(bis-(4-chlorophenyl)ethylene	2	0.0	75.5	44.3
1-chlorodibenzodioxin	1	0.0	61.3	50.0
1-chloronaphthalene	1	0.0	47.7	50.0
1-cis-3-pentadiene	1	0.5	42.6	53.7
1-cyclohexyl-1-phenyldodecane	1	12.5	127.6	142.3
1-decanethiol	1	8.0	134.3	109.1
1-decanol	1	8.0	134.5	109.1
1-decene	1	6.5	106.8	98.0
1-deoxy-D-glucopyranose	1	3.0	68.0	72.1
1-docosanol	1	21.0	185.6	205.0
1H-1,2,4-triazol-3-amine	1	0.0	51.2	50.0
1-heptanethiol	1	5.0	110.5	86.9
1-heptanol	1	5.0	75.5	86.9
1-heptene	1	3.5	81.9	75.8
1-hexacosanol	1	25.0	243.1	234.6
1-hexadecanol	1	15.0	181.2	160.7
1-hexadecene	1	13.0	124.4	146.0
1-hexanethiol	1	4.0	93.6	79.5
1-hexanol	1	4.0	68.6	79.5
1-hexene	1	2.5	70.1	68.5
1-iodonaphthalene	1	0.0	56.8	50.0
1-methoxy-2-(2,2,2-tricloro-1-(4-methoxyphenyl)ethyl) benzene	1	4.0	64.6	79.5
1-methyl-7-isopropylphenanthrene	1	1.0	48.9	57.4
1-methyl-9H-pyrido[3,4-b]indole	1	0.0	53.3	50.0
1-methylcyclohexanol	1	3.0	36.3	72.1
1-methylcyclopentanol	1	2.0	27.1	64.8
1-methylnaphthalene	1	0.0	49.3	50.0
1-methyltetrazole	1	0.0	49.8	50.0
1-naphthaleneacetamide	1	1.0	72.1	57.4
1-naphthaleneacetic acid	1	1.0	54.9	57.4
1-naphthoic acid	1	0.0	45.7	50.0

1-naphthyl benzoate	1	1.0	51.6	57.4
1-naphthyl methylcarbamate	1	2.0	58.9	64.8
1-naphthylamine	1	0.0	48.1	50.0
1-nitronaphthalene	1	0.0	55.9	50.0
1-nonanethiol	1	7.0	125.1	101.7
1-nonene	1	5.5	104.2	90.6
1-octanethiol	1	6.0	108.3	94.3
1-octene	1	4.5	89.3	83.2
1-pentadecanol	1	14.0	172.8	153.3
1-pentanethiol	1	3.0	88.8	72.1
1-pentanol	1	3.0	53.7	72.1
1-pentene	1	1.5	53.8	61.1
1-propanethiol	1	1.0	62.2	57.4
1-propanol	1	1.0	36.1	57.4
1-tetradecanol	1	13.0	158.6	146.0
1-undecene	1	7.5	118.2	105.4
2-((4-chloro-6-(cyclopropylamino)-1,3,5-triazin-2-yl) amino-2-methylpropanenitrile	1	2.5	51.3	68.5
2-(1,3-dioxolan-2-yl)phenyl methylcarbamate	1	2.5	61.5	68.5
2-(1'-cyclohexenyl)cyclohexanone	1	7.5	61.9	105.4
2-(1-methylethyl)phenyl methylcarbamate	1	3.0	70.8	72.1
2-(2,4,5-trichlorophenoxy)propanoic acid	1	2.0	87.8	64.8
2-(2,4-dichlorophenoxy)propanoic acid	1	2.0	78.2	64.8
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	1	1.0	74.4	57.4
2-(3-hydroxy-2-quinolinyl)-1H-indene-1,3(2H)-dione	1	0.0	57.3	50.0
2-(4-chloro-2-methylphenoxy)propanoic acid	1	2.0	72.2	64.8
2-(6-methoxy-2-naphthyl)propionic acid	1	2.0	67.0	64.8
2-(dimethylamino)-1,2-diphenylethanone	1	2.0	67.0	64.8
2-(docosanoxy)ethanol	1	24.0	171.5	227.2
2-(hexadecyloxy)ethanol	1	18.0	165.1	182.9
2,11-dicyclohexyldodecane	1	13.0	146.2	146.0
2,2,2-trinitroethanol	1	1.0	65.5	57.4
2,2,2-trinitroethyl 4,4,4-trinitrobutyrate	1	4.5	89.1	83.2
2,2,2-trinitroethyl-4,4-dinitropentanoate	1	6.5	73.0	98.0
2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	2	0.0	49.6	44.3
2,2',3,3',5,5',6,6'-octachlorobiphenyl	4	0.0	52.6	38.5
2,2',3,3',5,5',6-heptachlorobiphenyl	1	0.0	51.3	50.0
2,2',3,3',5,5'-hexachlorobiphenyl	2	0.0	68.7	44.3
2,2',3,3',6,6'-hexachlorobiphenyl	1	0.0	54.8	50.0
2,2,3,3-tetramethylbutane	6	0.0	33.3	35.1
2,2,3,3-tetramethylpentane	1	1.0	50.9	57.4
2,2,3-trimethylbutane	1	0.0	28.5	50.0
2,2',4,4',6,6'-hexachlorobiphenyl	4	0.0	45.3	38.5
2,2,4,4-tetramethylpentan-3-ol	1	0.0	29.9	50.0
2,2,4,4-tetramethylpentane	1	0.0	47.2	50.0
2,2',4,5,5'-pentachlorobiphenyl	1	0.0	53.7	50.0
2,2',4',5-tetrachlorobiphenyl	1	0.0	69.0	50.0
2,2,4-trimethylpentane	1	1.0	55.5	57.4
2,2,5,5-tetramethylhex-3-ene	1	0.0	61.0	50.0
2,2,6,6-tetramethyl-1,3-dioxane	1	3.0	43.5	72.1
2,2-bis-(4-cyanatophenyl)propane	1	3.0	75.0	72.1
2,2-bis(phenylthio)propane	1	3.0	74.2	72.1

2,2-bis-hydroxymethylpropanoic acid	1	2.5	98.1	68.5
2,2-dichloropropane	1	0.0	41.4	50.0
2,2-dicyanopropane	1	0.0	45.3	50.0
2,2-dimethoxy-1,2-diphenylethanone	1	3.0	61.6	72.1
2,2-dimethyl-1,3-dioxan	1	3.0	52.7	72.1
2,2-dimethyl-1,3-propanediol	1	1.0	55.2	57.4
2,2-dimethyl-1-propanol	1	0.0	31.1	50.0
2,2-dimethylbutane	1	0.0	45.9	50.0
2,2-dimethylheptane	1	3.0	76.1	72.1
2,2-dimethylpentane	1	1.0	39.6	57.4
2,2-dimethylpropane	12	0.0	31.1	29.4
2,2-dimethylpropanoic acid (pivalic acid)	1	0.0	36.7	50.0
2,2-dinitro-1,3-propanediol	1	2.0	62.5	64.8
2,2-dinitropropane	1	0.0	57.2	50.0
2,2-dinitropropanol	1	1.0	61.2	57.4
2,2-dinitropropyl-4,4-dinitropentanoate	1	6.5	86.5	98.0
2,2-dintropropyl-4,4,4-trinitrobutyrate	1	5.5	171.8	90.6
2,2'-methylenebis(3,4,6-trichlorophenol)	1	1.0	76.0	57.4
2,3,4,5,6-pentachlorobiphenyl	2	0.0	53.7	44.3
2,3,4,5,6-pentafluorotoluene	2	0.0	54.5	44.3
2,3,4,5-tetrachlorobiphenyl	1	0.0	69.2	50.0
2,3,4-trimethylpentane	1	2.0	56.7	64.8
2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione	4	0.0	54.4	38.5
2,3,5-tricarbomethoxynaphthalene	1	3.0	102.1	72.1
2,3,5-triiodobenzoic acid	1	0.0	64.0	50.0
2,3,6,7,10,11-hexakis(1-decynyl)triphenylene	1	42.0	200.5	360.0
2,3,6,7-tetracarbomethoxynaphthalene	1	4.0	92.1	79.5
2,3,6-tricarbomethoxynaphthalene	1	3.0	86.2	72.1
2,3,6-trichlorobenzoic acid	1	0.0	59.2	50.0
2,3,6-trichlorophenylacetic acid	1	1.0	51.9	57.4
2,3-benzofluorene	1	0.0	47.8	50.0
2,3-dicarbomethoxynaphthalene	1	2.0	62.3	64.8
2,3-dichloro-1,4-naphthalenedione	2	0.0	60.8	44.3
2,3-dichlorophenol	1	0.0	64.7	50.0
2,3-dihydro-2,2-dimethyl-7-benzofuranol-3-one	1	0.0	49.5	50.0
2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	1	2.0	71.2	64.8
2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	1	2.5	66.4	68.5
2,3-dimethyl-2,3-bis(4-tert-butylphenyl)butane	1	2.0	89.1	64.8
2,3-dimethyl-2,3-bis(phenylazo)butane	1	2.0	61.6	64.8
2,3-dimethyl-2,3-butanediol	1	1.0	46.5	57.4
2,3-dimethyl-2,3-diphenylbutane	1	2.0	65.1	64.8
2,3-dimethyl-2-butene	4	0.0	50.1	38.5
2,3-dimethylbenzoic acid	1	0.0	43.8	50.0
2,3-dimethylbutane	1	1.0	53.0	57.4
2,3-dimethylnaphthalene	2	0.0	42.1	44.3
2,3-dimethylphenol	1	0.0	60.8	50.0
2,3-dimethylpyridine	1	0.0	52.1	50.0
2,3-dinitrophenol	1	0.0	62.9	50.0
2,3-dinitrotoluene	1	0.0	53.3	50.0
2,3-pentadiene	20	0.0	44.8	25.2
2,4,4-trimethyl-1-pentene	1	0.5	49.1	53.7

2,4,4-trimethyl-2-pentene	1	0.0	40.8	50.0
2,4,5,6-tetrachloro-1,3-benzenedicarbonitile	2	0.0	57.0	44.3
2,4,5-tribromostyrene	1	0.0	73.8	50.0
2,4,5-trichlorobiphenyl	1	0.0	65.2	50.0
2,4,5-trichlorophenol	1	0.0	63.4	50.0
2,4,5-trimethylthiazole	1	0.0	37.4	50.0
2,4,5-trinitrotoluene	1	0.0	65.7	50.0
2,4,6,N-tetranitro-N-methyltoluidene	1	0.5	51.5	53.7
2,4,6-N-tetranitroethylaniline	1	1.5	63.7	61.1
2,4,6-tribromophenol	1	0.0	50.6	50.0
2,4,6-trichlorobiphenyl	2	0.0	49.4	44.3
2,4,6-trimethyl-1,3,5-trioxane	1	0.0	54.4	50.0
2,4,6-trimethylpyridine	1	0.0	41.7	50.0
2,4,6-trinitro-1,3-dimethylbenzene	1	0.0	84.5	50.0
2,4,6-trinitroresorcinol	1	0.0	73.7	50.0
2,4,6-trinitrotoluene	2	0.0	66.5	44.3
2,4,6-tri-tert-butylphenol	1	0.0	48.0	50.0
2,4,7-trinitrofluoren-9-one	1	3.0	58.8	72.1
2,4-dibromophenol	1	0.0	46.8	50.0
2,4-dichlorophenol	1	0.0	63.2	50.0
2,4-dichlorophenyl 4-nitrophenyl ether	1	1.0	67.1	57.4
2,4-dimethylpentane	1	2.0	44.5	64.8
2,4-dimethylpyridine	1	0.0	42.1	50.0
2,4-dimethylpyrrole	1	0.0	35.8	50.0
2,4-dimethylthiazole	2	0.0	13.0	44.3
2,4-dinitrochlorobenzene	1	0.0	62.0	50.0
2,4-dinitrophenol	1	0.0	62.3	50.0
2,4-dinitrotoluene	1	0.0	58.6	50.0
2,4-di-tert-butylthiazole	1	0.0	40.7	50.0
2,4-hexadiyne	20	0.0	8.5	25.2
2,5,8,11-tetraoxadodecane	1	9.0	103.4	116.4
2,5,8-trioxanonane	1	6.0	85.0	94.3
2,5-dibutoxy-1,4-benzoquinone	1	7.5	87.2	105.4
2,5-dichlorophenol	1	0.0	67.8	50.0
2,5-diethoxy-1,4-benzoquinone	1	3.5	62.5	75.8
2,5-dimethylaniline	1	0.0	49.1	50.0
2,5-dimethylphenol	1	0.0	67.2	50.0
2,5-dimethylpyridine	1	0.0	56.5	50.0
2,5-dimethylpyrrole	2	0.0	33.1	44.3
2,5-dimethyltetrazole	1	0.0	52.7	50.0
2,5-dimethylthiophene	2	0.0	42.3	44.3
2,5-di-n-heptadecyloxy-1,4-benzoquinone	1	34.0	339.7	301.0
2,5-di-n-heptyloxy-1,4-benzoquinone	1	14.0	154.0	153.3
2,5-di-n-hexadecyloxy-1,4-benzoquinone	1	32.0	316.1	286.2
2,5-di-n-hexyloxy-1,4-benzoquinone	1	11.5	110.3	134.9
2,5-dinitrophenol	1	0.0	62.3	50.0
2,5-di-n-nonadecyloxy-1,4-benzoquinone	1	38.0	380.2	330.5
2,5-di-n-nonyloxy-1,4-benzoquinone	1	18.0	202.7	182.9
2,5-di-n-octyloxy-1,4-benzoquinone	1	16.0	132.2	168.1
2,5-di-n-pentadecyloxy-1,4-benzoquinone	1	30.0	328.5	271.5
2,5-di-n-undecyloxy-1,4-benzoquinone	1	22.0	239.1	212.4
2,5-dipentoxy-1,4-benzoquinone	1	9.5	115.0	120.1
2,5-dipropoxy-1,4-benzoquinone	1	5.5	97.0	90.6

2,6-dichloro-4-benzenamine	2	0.0	63.1	44.3
2,6-dichloro-4-nitroaniline	2	0.0	69.9	44.3
2,6-dichlorobenzonitrile	2	0.0	62.7	44.3
2,6-dichlorobiphenyl	2	0.0	40.9	44.3
2,6-dichlorophenol	2	0.0	65.1	44.3
2,6-diisopropylphenol	1	1.5	50.0	61.1
2,6-dimethylnaphthalene	2	0.0	65.4	44.3
2,6-dimethylphenol	2	0.0	59.3	44.3
2,6-dimethylpyridine	2	0.0	48.8	44.3
2,6-dinitrochlorobenzene	1	0.0	52.5	50.0
2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	1	8.0	69.4	109.1
2,6-dinitrophenol	1	0.0	58.3	50.0
2,6-dinitrotoluene	1	0.0	72.8	50.0
2,6-di-tert-butyl-4-methoxyphenol	1	0.5	71.8	53.7
2,6-di-tert-butyl-4-methylphenol	1	0.0	69.4	50.0
2,6-di-tert-butylphenol	1	0.0	53.3	50.0
2,7-dicarbomethoxynaphthalene	1	2.0	64.8	64.8
2,7-dimethylnaphthalene	2	0.0	63.3	44.3
2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	1	0.5	78.1	53.7
2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	1	2.0	79.8	64.8
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	1	3.5	95.8	75.8
2-[bis(2-chloroethyl)amino]tetrahydro-2H-1,3,2-oxazophosphorine-2-oxide	1	6.5	102.7	98.0
2-acetoxynaphthalene	1	1.0	58.6	57.4
2-acetyl-1-naphthol	1	0.0	60.6	50.0
2-acetylamino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	1	5.0	109.8	86.9
2-acetylamino-9-[(2-hydroxyethoxy)methyl]-9H-purine	1	5.0	120.9	86.9
2-amino-2-hydroxymethylpropane-1,3-diol	1	3.0	87.5	72.1
2-amino-2-methylpropane-1,3-diol	1	2.0	79.4	64.8
2-amino-9-[(2-acetoxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	1	4.0	96.9	79.5
2-amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	1	3.5	57.6	75.8
2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	1	3.5	91.3	75.8
2-aminobenzoic acid	1	0.0	49.1	50.0
2-aminobiphenyl	1	0.0	43.4	50.0
2-aminopropane	1	0.0	41.2	50.0
2-benzoyl-1-naphthol	1	0.0	58.7	50.0
2-bromo-2-chloro-1,1,1-trifluoroethane	1	0.0	31.3	50.0
2-bromobutane	1	1.0	42.9	57.4
2-bromonaphthalene	1	0.0	61.9	50.0
2-bromopropane	1	0.0	35.6	50.0
2-bromothiophene	1	0.0	38.8	50.0
2-butanethiol	1	1.0	48.7	57.4
2-butanol	1	1.0	32.3	57.4
2-butanone	1	0.5	45.3	53.7
2-butyne	20	0.0	38.4	25.2
2-carbomethoxynaphthalene	1	1.0	77.4	57.4
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	1	5.0	83.8	86.9

2-chloro-2-nitropropane	1	0.0	49.7	50.0
2-chloro-6-(trichloromethyl)pyridine	1	0.0	60.1	50.0
2-chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene	1	3.0	75.1	72.1
2-chloroanthraquinone	1	0.0	80.7	50.0
2-chlorobenzoic acid	1	0.0	62.2	50.0
2-chlorobiphenyl	1	0.0	47.7	50.0
2-chlorodibenzodioxin	1	0.0	63.8	50.0
2-chloroethylphosphonic acid	1	1.0	42.5	57.4
2-chloro-n-(2,6-diethylphenyl)-n-(methoxymethyl) acetamide	1	6.0	80.1	94.3
2-chloronaphthalene	1	0.0	44.3	50.0
2-chloro-N-isopropyl N-phenylacetamide	1	3.0	74.1	72.1
2-chloro-N-isopropylacetamide	1	2.5	74.2	68.5
2-chlorophenol	1	0.0	44.6	50.0
2-chloropropane	1	0.0	47.4	50.0
2-chlorothiophene	1	0.0	44.6	50.0
2-cyano-2-methylpropane	1	0.0	39.1	50.0
2-cyclohexyl-4,6-dinitrophenol	1	2.5	74.0	68.5
2-cyclohexylcyclohexanone	1	8.5	65.0	112.7
2-deoxy-2-fluoro-D-glucopyranose	1	3.0	89.4	72.1
2-deoxy-D-glucopyranose	1	3.0	86.5	72.1
2-ethoxyisonitrosoacetanilide	1	4.0	56.8	79.5
2-ethyl-2-diphenylmethyl-1,3-cyclopentanedione	1	1.5	73.8	61.1
2-fluorenyl-2-methyl-1,3-cyclohexanedione	1	1.0	79.7	57.4
2-fluorenyl-2-methyl-1,3-cyclopentanedione	1	0.5	62.2	53.7
2-fluorotoluene	1	0.0	46.5	50.0
2-heneicosanone	1	18.0	232.6	182.9
2-heptanone	1	3.5	82.9	75.8
2-hexadecanoyloxy-1,3-bis-(9-cis-octadecenoyloxy) propane	1	48.0	429.9	404.3
2-hexanone	1	2.5	68.4	68.5
2-hydroxybenzoic acid	1	0.0	57.0	50.0
2-hydroxymethyl-2-methyl-1,3-propanediol	1	2.0	76.9	64.8
2-iodobenzoic acid	1	0.0	49.1	50.0
2-iodonaphthalene	1	0.0	49.0	50.0
2-isopropoxyphenyl N-methylcarbamate	1	4.0	63.2	79.5
2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide	1	0.5	51.6	53.7
2-methyl-1,3-butadiene	1	0.0	38.6	50.0
2-methyl-1-butene	1	0.5	58.3	53.7
2-methyl-1-phenyl-2-(N-piperidinyl)-1-propanone	1	4.0	54.0	79.5
2-methyl-1-propanol	1	1.0	36.9	57.4
2-methyl-2-(methylsulfonyl)propanal oxime	1	1.0	71.0	57.4
2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime	1	4.5	60.7	83.2
2-methyl-2-butanethiol	1	2.0	52.5	64.8
2-methyl-2-butanol	1	2.0	31.1	64.8
2-methyl-2-butene	1	0.0	54.4	50.0
2-methyl-2-diphenylmethyl-1,3-cyclopentanedione	1	2.5	87.0	68.5
2-methyl-2-nitro-1,3-propandiol	1	2.0	82.1	64.8
2-methyl-2-nitro-1-propanol	1	1.0	65.8	57.4
2-methyl-2-nitropropyl-4,4,4-trinitrobutyrate	1	5.5	85.7	90.6
2-methyl-4,6-dinitrophenol	1	0.0	54.0	50.0

2-methylbutane	1	1.0	45.2	57.4
2-methylcyclothiapentane	1	2.0	51.5	64.8
2-methyldecane	1	7.0	111.7	101.7
2-methylfuran	1	0.0	47.0	50.0
2-methylheptane	1	4.0	72.6	79.5
2-methylhexane	1	3.0	59.3	72.1
2-methylnaphthalene	1	0.0	58.9	50.0
2-methylnonane	1	6.0	88.0	94.3
2-methylpentane	1	2.0	52.4	64.8
2-methylpiperidine	1	3.0	69.0	72.1
2-methylpyridine	1	0.0	47.1	50.0
2-methyltetrazole	1	0.0	43.3	50.0
2-methylthiazole	1	0.0	48.9	50.0
2-methylthiophene	1	0.0	45.6	50.0
2-naphthoic acid	1	0.0	51.2	50.0
2-naphthyl benzoate	1	1.0	68.8	57.4
2-naphthylamine	1	0.0	60.4	50.0
2-n-butyl-5-(4-bromobiphenyl-4-yl)thiophene	1	3.5	42.7	75.8
2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	1	4.0	50.6	79.5
2-nitro-5-methylphenol	1	0.0	68.7	50.0
2-nitroaniline	1	0.0	46.8	50.0
2-nonadecanone	1	16.0	209.3	168.1
2-n-propyl-5-(4-bromophenyl)thiophene	1	2.0	43.6	64.8
2-octanone	1	4.5	96.6	83.2
2-pentadecanone	1	12.0	174.2	138.6
2-pentanol	1	2.0	42.4	64.8
2-pentanone	1	1.5	56.3	61.1
2-phenylbenzimidazole	2	0.0	38.8	44.3
2-piperadone	1	2.5	47.0	68.5
2-propanethiol	1	0.0	40.5	50.0
2-propanol	1	0.0	29.2	50.0
2-pyrrolidone	1	1.5	46.6	61.1
2-sec-butyl-4,6-dinitrophenol	1	1.5	69.5	61.1
2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate	1	5.0	55.3	86.9
2-tetradecanone	1	11.0	160.2	131.2
2-undecanone	1	7.5	99.1	105.4
3-(1-methylethyl)-(1H)-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide	1	0.5	52.8	53.7
3-(3,4-dichlorophenyl)-1,1-dimethylurea	1	2.0	78.9	64.8
3-(4-chlorophenyl)-1,1-dimethylurea	1	2.0	65.8	64.8
3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	1	1.5	62.3	61.1
3(n-decylamino)-1,2-propanediol	1	13.0	158.1	146.0
3(n-decyloxy)-1,2-propanediol	1	13.0	125.1	146.0
3(n-decylthio)-1,2-propanediol	1	13.0	114.7	146.0
3(n-dodecylamino)-1,2-propanediol	1	15.0	176.5	160.7
3(n-dodecyloxy)-1,2-propanediol	1	15.0	159.1	160.7
3(n-dodecylthio)-1,2-propanediol	1	15.0	122.9	160.7
3(n-heptylamino)-1,2-propanediol	1	9.0	88.6	116.4
3(n-heptyloxy)-1,2-propanediol	1	9.0	104.1	116.4
3(n-heptylthio)-1,2-propanediol	1	9.0	100.1	116.4
3(n-hexyloxy)-1,2-propanediol	1	8.0	37.4	109.1
3(n-hexylthio)-1,2-propanediol	1	8.0	166.8	109.1

3(n-nonylamino)-1,2-propanediol	1	11.0	155.0	131.2
3-(n-nonyloxy)-1,2-propanediol	1	11.0	99.3	131.2
3(n-octylamino)-1,2-propanediol	1	10.0	134.3	123.8
3(n-octyloxy)-1,2-propanediol	1	10.0	112.8	123.8
3(n-octylthio)-1,2-propanediol	1	10.0	129.9	123.8
3(n-tetradecylamino)-1,2-propanediol	1	17.0	182.2	175.5
3(n-tetradecyloxy)-1,2-propanediol	1	17.0	187.4	175.5
3(n-tetradecylthio)-1,2-propanediol	1	17.0	133.6	175.5
3(n-tridecylamino)-1,2-propanediol	1	16.0	193.6	168.1
3(n-tridecyloxy)-1,2-propanediol	1	16.0	158.5	168.1
3(n-tridecylthio)-1,2-propanediol	1	16.0	106.7	168.1
3(n-undecylamino)-1,2-propanediol	1	14.0	166.9	153.3
3(n-undecyloxy)-1,2-propanediol	1	14.0	138.3	153.3
3(n-undecylthio)-1,2-propanediol	1	14.0	99.1	153.3
3-(p-tolyl-4-sulfonyl)-1-butyl urea	1	5.0	63.3	86.9
3,3',4'4'-tetraaminodiphenyl ether	1	1.0	62.8	57.4
3,3',5,5'-tetra-tert-butyldiphenylmethane-4,4'-diol	1	5.0	96.0	86.9
3,3'-bis-(1-cyclohexylethyl)-5,5'-dimethyldiphenyl methane-2,2'-diol	1	10.0	73.1	123.8
3,3-bis-(chloromethyl)oxacyclobutane	1	2.0	58.0	64.8
3,3-diethylpentane	1	4.0	48.2	79.5
3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime	1	4.5	60.1	83.2
3,3-dimethyl-1-butene	1	0.0	41.7	50.0
3,3-dimethyl-2-butanone	1	0.0	51.2	50.0
3,3-dimethylpentane	1	2.0	51.2	64.8
3,3-dimethylpentanedioic anhydride	2	0.0	45.4	44.3
3,3'-di-tert-butyl-5,5'-dimethyl-2,2-dihydroxydiphenyl methane	1	3.0	72.7	72.1
3,4-benzophenanthrene	1	0.0	48.8	50.0
3,4-benzopyrene	1	0.0	59.9	50.0
3,4-dichloro-2-methoxybenzoic acid	1	1.0	85.6	57.4
3,4-dichlorophenol	1	0.0	61.4	50.0
3',4'-dichloropropionanilide	1	2.0	50.2	64.8
3,4-diethyl-3,4-bis(4-tert-butylphenyl)hexane	1	8.0	74.3	109.1
3,4-dimethylisoxazol 5-sulphanylamide	1	1.0	62.5	57.4
3,4-dimethylphenol	1	0.0	54.3	50.0
3,4-dimethylphenyl methylcarbamate	1	2.0	71.2	64.8
3,4-dimethylpyridine	1	0.0	56.0	50.0
3,4-dinitrophenol	1	0.0	62.3	50.0
3,4-dinitrotoluene	1	0.0	57.1	50.0
3,5,6-trichloro-2-pyridinol	1	0.0	57.6	50.0
3,5,6-trichloro-2-pyridinyloxyacetic acid	1	2.0	73.6	64.8
3,5-dibromo-4-hydroxybenzonitrile	2	0.0	69.0	44.3
3,5-dichlorobenzoic acid	2	0.0	50.0	44.3
3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	1	2.0	66.9	64.8
3,5-dichlorophenol	2	0.0	60.1	44.3
3,5-diisopropylphenol	1	1.5	37.2	61.1
3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate	1	3.0	50.8	72.1
3,5-dimethylbenzoic acid	2	0.0	51.0	44.3
3,5-dimethylphenol	2	0.0	53.4	44.3
3,5-dimethylpyridine	2	0.0	49.1	44.3
3,5-dinitrobenzoic acid	1	0.0	47.5	50.0

3,6-dichloro-2-methoxybenzoic acid	1	1.0	59.2	57.4
3,6-dichloro-5-hydroxy-2-methoxybenzoic acid	1	1.0	70.7	57.4
3-amino-2,5-dichlorobenzoic acid	1	0.0	78.7	50.0
3-aminoacetophenone	1	0.0	78.1	50.0
3-aminobenzoic acid	1	0.0	48.2	50.0
3-bromopentane	1	2.0	50.2	64.8
3-chloro-1,1,1,3,3-pentafluoropropane	1	0.0	63.3	50.0
3-chlorobenzoic acid	1	0.0	55.8	50.0
3-chlorophenol	1	0.0	48.8	50.0
3-deoxy-3-fluoro-D-glucopyranose	1	3.0	48.4	72.1
3-deoxy-D-glucopyranose	1	3.0	84.2	72.1
3-diphenylmethyl-2,4-pentanedione	1	2.0	69.8	64.8
3-ethyl-3-diphenylmethyl-2,4-pentanedione	1	3.0	89.4	72.1
3-ethylheptane	1	5.0	101.4	86.9
3-ethylpentane	1	3.0	61.8	72.1
3-fluorotoluene	1	0.0	45.1	50.0
3-heptanone	1	3.5	74.3	75.8
3-hexanone	1	2.5	66.6	68.5
3-hydroxybenzoic acid	1	0.0	55.1	50.0
3-iodobenzoic acid	1	0.0	62.3	50.0
3-methyl-1,2-butadiene	2	0.0	49.8	44.3
3-methyl-1-butanethiol	1	2.0	53.1	64.8
3-methyl-1-butene	1	0.5	51.2	53.7
3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	1	2.0	66.0	64.8
3-methyl-2-butanethiol	1	1.0	52.5	57.4
3-methyl-3-diphenylmethyl-2,4-pentanedione	1	2.0	71.3	64.8
3-methylcyclothiapentane	1	2.0	54.0	64.8
3-methylheptane	1	4.0	76.5	79.5
3-methylpentane	1	2.0	48.1	64.8
3-methylpyridine	1	0.0	55.6	50.0
3-methylthiophene	1	0.0	51.6	50.0
3-nitroaniline	1	0.0	61.2	50.0
3-nitrophthalic anhydride	1	0.0	42.2	50.0
3-nitrotoluene	1	0.0	51.9	50.0
3-pentanol	1	2.0	44.5	64.8
3-pentanone	1	1.5	50.0	61.1
3-propyl-3-diphenylmethyl-2,4-pentanedione	1	4.0	77.6	79.5
4-(1,1-dimethylethyl)-n-(1-methylpropyl)-2,6-dinitrobenzeneamine	1	6.0	61.5	94.3
4-(2,4,5-trichlorophenoxy)butanoic acid	1	4.0	78.3	79.5
4-(2,4-dichlorophenoxy)butyric acid	1	4.0	98.2	79.5
4-(2-chlorophenylhydrazone)-3-methyl-5-isoxazolone	1	1.5	63.7	61.1
4-(4-chloro-2-methylphenoxy)butanoic acid	1	4.0	85.8	79.5
4-(4-nitrophenylazo)aniline	1	1.0	65.3	57.4
4-(6-hexenyloxy)-3',4'difluorodiphenyldiacetylene	1	5.0	101.2	86.9
4-(cis-3-hexenyloxy)-3',4'difluorodiphenyldiacetylene	1	4.0	84.9	79.5
4-(cis-4-hexenyloxy)-3',4'difluorodiphenyldiacetylene	1	4.0	96.9	79.5
4-(dipropylamino)-N,N-dimethyl-3,5-dinitrobenzenesulfonamide	1	6.0	78.7	94.3
4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide	1	4.5	92.8	83.2
4,4'-di-(2-methoxyethoxy)biphenyl	1	8.0	97.5	109.1
4,4'dichlorodiphenylsulphone	1	0.0	57.8	50.0
4,4'-didecanoyloxydiphenyldiacetylene	1	18.0	250.5	182.9

4,4'-didodecanoyloxydiphenyldiacetylene	1	22.0	244.0	212.4
4,4'dihydroxydiphenyl-2,2-propane	1	1.0	69.5	57.4
4,4'-dinitrodiphenyl ether	1	1.0	24.6	57.4
4,4'-diundecanoyloxydiphenyldiacetylene	1	20.0	165.3	197.6
4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	1	1.0	73.0	57.4
4[p-[bis(2-chloroethyl)amino]benzene]butanoic acid	1	8.0	86.1	109.1
4'4'-diaminodiphenyl ether	1	1.0	16.6	57.4
4-acetoxybenzoic acid	1	1.5	56.4	61.1
4-amino-6-(1,1-dimethylethyl)-3-(methylthio) 1,2,4-triazin-5(4H)-one	1	0.5	45.1	53.7
4-aminoacetophenone	1	0.0	100.2	50.0
4-aminobenzoic acid	2	0.0	45.3	44.3
4-amino-N-(6-methoxy-3-pyridazinyl) benzenesulfonamide	1	2.0	49.2	64.8
4-aminopyridine	2	0.0	46.7	44.3
4-benzoyl-1-naphthol	1	0.0	65.0	50.0
4-bromo-2,5-dichloroaniline	1	0.0	64.4	50.0
4-bromo-2,5-dichlorophenol	1	0.0	64.4	50.0
4-chloroazobenzene	2	0.0	75.3	44.3
4-chlorobenzoic acid	2	0.0	62.9	44.3
4-chlorobiphenyl	2	0.0	38.2	44.3
4-chlorobut-2-ynyl 3-chlorophenylcarbamate	1	4.0	78.2	79.5
4-chlorophenol	2	0.0	44.5	44.3
4-chlorophenoxyacetic acid	1	2.0	84.4	64.8
4-chlorophenyl 4-chlorobenzenesulfonate	1	1.0	65.6	57.4
4-chlorophenylbenzenesulfonate	1	1.0	64.5	57.4
4-ethoxy-4'fluorodiphenyldiacetylene	1	2.0	84.7	64.8
4-ethoxy-4'-trifluoromethyldiphenyldiacetylene	1	3.0	77.0	72.1
4-ethoxybenzoic acid	1	2.0	62.2	64.8
4-ethoxyisonitrosoacetanilide	1	4.0	15.5	79.5
4-ethoxyphenylacetic acid	1	3.0	63.9	72.1
4-ethylbenzoic acid	1	1.0	36.4	57.4
4-ethynyl-1-[(4-ethynylphenyl)methoxy]benzene	1	2.0	57.1	64.8
4-fluorotoluene	2	0.0	43.2	44.3
4-heptanone	1	3.5	67.3	75.8
4-hexylresorcinol	1	4.5	55.8	83.2
4-hydroxy-3,5-diiodobenzonitrile	2	0.0	69.6	44.3
4-hydroxyazobenzene	2	0.0	77.6	44.3
4-hydroxybenzoic acid	2	0.0	63.3	44.3
4-hydroxyphenylacetic acid	1	1.0	67.0	57.4
4-hydroxyphenylpropionic acid	1	2.0	71.8	64.8
4-iodobenzoic acid	2	0.0	64.8	44.3
4-methoxybenzoic acid	1	1.0	62.0	57.4
4-methoxyphenol	1	0.5	55.7	53.7
4-methoxyphenylacetic acid	1	2.0	60.9	64.8
4-methoxyphenylbutyric acid	1	4.0	76.5	79.5
4-methoxyphenylpropionic acid	1	3.0	75.6	72.1
4-methyl-7-aminocoumarin	1	0.0	64.2	50.0
4-methyl-7-diethylaminocoumarin	1	3.0	52.0	72.1
4-methyl-7-dimethylaminocoumarin	1	0.5	57.5	53.7
4-methyl-7-hydroxycoumarin	1	0.0	63.3	50.0
4-methylcyclohex-1-ene	1	2.0	43.2	64.8
4-methylheptane	1	4.0	71.2	79.5

4-methylpent-1-ene	1	1.5	41.5	61.1
4-methylphenanthrene	1	0.0	43.4	50.0
4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline	1	5.0	66.1	86.9
4-methylthiazole	1	0.0	38.8	50.0
4-methylthio-3,5-xylyl methylcarbamate	1	3.0	77.1	72.1
4-n-butoxy-2',3',4'-trifluorodiphenylacetylene	1	4.0	104.5	79.5
4-n-butoxy-4'-fluorodiphenylacetylene	1	4.0	73.3	79.5
4-n-butoxy-4'-trifluoromethyldiphenyldiacetylene	1	5.0	61.2	86.9
4-n-butoxybenzoic acid	1	4.0	51.5	79.5
4-n-butyl-3',4'-difluorodiphenylacetylene	1	3.0	78.2	72.1
4-n-butyl-3',4'-difluorodiphenyldiacetylene	1	3.0	71.4	72.1
4-n-butyl-4'-fluorodiphenylacetylene	1	3.0	56.1	72.1
4-n-ethoxy-2',3',4'-trifluorodiphenylacetylene	1	2.0	90.2	64.8
4-n-ethoxy-2',4'-difluorodiphenylacetylene	1	2.0	78.6	64.8
4-n-ethoxy-4'-fluorodiphenylacetylene	1	2.0	64.3	64.8
4-n-ethyl-3',4'-difluorodiphenylacetylene	1	1.0	55.1	57.4
4-n-hexyl-3',4'-difluorodiphenylacetylene	1	5.0	77.2	86.9
4-n-hexylbenzoic acid	1	5.0	53.2	86.9
4-n-hexyloxy-2',3',4'-trifluorodiphenylacetylene	1	6.0	95.7	94.3
4-n-hexyloxy-2',4'-difluorodiphenylacetylene	1	6.0	106.3	94.3
4-n-hexyloxy-3',4'-difluorodiphenylacetylene	1	6.0	102.3	94.3
4-n-hexyloxy-4'-trifluoromethyldiphenyldiacetylene	1	7.0	86.1	101.7
4-nitro-4'-methylbenzylidene aniline	1	1.0	67.9	57.4
4-nitro-5-methylphenol	1	0.0	68.3	50.0
4-nitroaniline	2	0.0	50.2	44.3
4-nitrophthalic anhydride	1	0.0	44.2	50.0
4-nitrotoluene	2	0.0	51.8	44.3
4-n-octyloxy-N-(3,5-dimethoxybenzylidene)aniline	1	10.0	111.6	123.8
4-n-octyloxy-N-(3,5-dimethylbenzylidene)aniline	1	8.0	116.2	109.1
4-n-octyloxy-N-(4-methoxybenzylidene)aniline	1	9.0	112.1	116.4
4-n-pentoxy-2',3',4'-trifluorodiphenylacetylene	1	5.0	104.8	86.9
4-n-pentoxy-4'-fluorodiphenylacetylene	1	5.0	82.2	86.9
4-n-pentoxybenzoic acid	1	5.0	59.7	86.9
4-n-pentyl-3',4'-difluorodiphenylacetylene	1	4.0	68.4	79.5
4-n-pentyl-3',4'-difluorodiphenyldiacetylene	1	4.0	86.9	79.5
4-n-pentyl-4'-fluorodiphenylacetylene	1	4.0	75.9	79.5
4-n-pentylbenzoic acid	1	4.0	41.5	79.5
4-n-propoxy-2',3',4'-trifluorodiphenylacetylene	1	3.0	79.7	72.1
4-n-propoxy-2',4'-difluorodiphenylacetylene	1	3.0	77.1	72.1
4-n-propoxy-4'-fluorodiphenylacetylene	1	3.0	76.0	72.1
4-n-propoxybenzoic acid	1	3.0	65.9	72.1
4-n-propyl-3',4'-difluorodiphenylacetylene	1	2.0	65.0	64.8
4-n-propyl-3',4'difluorodiphenyldiacetylene	1	2.0	64.1	64.8
4-n-propyl-4'-fluorodiphenylacetylene	1	2.0	74.4	64.8
4-octadecynoic acid	1	14.0	166.5	153.3
4-oxaheptane	1	4.0	68.0	79.5
4-propoxy-4'-trifluoromethyldiphenyldiacetylene	1	4.0	59.5	79.5
4-propylbenzoic acid	1	2.0	66.5	64.8
4'-propylbiphenyl-4-carbonitrile	1	2.0	67.0	64.8
4-tert-butylbenzoic acid	1	0.0	40.7	50.0
4-tert-butylphenol	1	0.0	38.9	50.0
4-trans-(3-fluoro-4-cyanophenyl)cyclohexyl (E)-but-2-enoate	1	5.0	53.7	86.9

4-trans-(4-bromophenyl)cyclohexyl (E)-2-butenoate	1	5.0	73.2	86.9
4-trans-(4-chlorophenyl)cyclohexyl (E)-2-butenoate	1	5.0	78.2	86.9
4-trans-(4-fluorophenyl)cyclohexyl (E)-2-butenoate	1	5.0	70.9	86.9
4-trans-(4-fluorophenylethyl)cyclohexyl (E)-butenoate	1	7.0	74.6	101.7
4-trans-(trifluoromethoxyphenyl)cyclohexyl (E)-but-2-enoate	1	6.0	63.5	94.3
4-trans-cyanocyclohexyl (E) 2-butenoate	1	4.5	66.6	83.2
5'-(trifluoromethanesulphonamide)acet-2',4-xylidide	1	2.0	82.4	64.8
5,5-bis(3,3-dimethylbutyl)2,2,8,8-tetramethylnonane	1	13.0	102.7	146.0
5,5-dimethylperhydro-1,3-oxazine-2-one	1	2.5	64.8	68.5
5,6,7,8-tetrahydroquinoline	1	1.0	40.8	57.4
5,6-dibutyl-5,6-bis(4-tert-butylphenyl)decane	1	16.0	111.7	168.1
5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid	1	3.0	86.3	72.1
5-amino-4-chloro-2-phenyl-3(2H)-pyridazinone	1	1.5	55.8	61.1
5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione	1	1.5	51.4	61.1
5-butyl-2-ethylamino-6-methylpyrimidin-4-ol	1	4.5	47.0	83.2
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	1	0.0	27.9	50.0
5-isopropyl-m-tolyl methylcarbamate	1	3.0	63.8	72.1
5-methyl N-(methylcarbamoyloxy)thioacetimidate	1	3.5	61.6	75.8
5-methyl-1,2,4-triazolo[3,4-b]benzothiazole	1	0.0	52.3	50.0
5-methylnonane	1	6.0	89.2	94.3
5-methyltetrazole	2	0.0	38.3	44.3
5-methylthiazole	1	0.0	32.9	50.0
5-nonanone	1	5.5	117.5	90.6
5-octadecynoic acid	1	14.0	167.4	153.3
6-(4-biphenyl)-1-hexene	1	4.0	55.0	79.5
6,8,9-trimethyladenine	1	0.5	52.7	53.7
6,9-dimethyl-8-butyladenine	1	3.5	88.0	75.8
6-deoxy-6-fluoro-D-glucopyranose	1	3.0	66.0	72.1
6-deoxy-D-glucopyranose	1	3.0	55.5	72.1
6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one	1	0.0	67.5	50.0
6-octadecynoic acid	1	14.0	169.5	153.3
7,8-benzoquinoline	1	0.0	43.5	50.0
7-octadecynoic acid	1	14.0	166.5	153.3
8-(4-biphenyl)-1-octene	1	6.0	72.0	94.3
8-[4-(4'-n-butylbiphenyl)]-1-octene	1	9.0	39.3	116.4
8-octadecynoic acid	1	14.0	172.8	153.3
9-fluorenone	2	0.0	50.8	44.3
9-heptadecanone	1	14.0	205.9	153.3
9H-pyrido[3,4-b]indole	1	0.0	54.1	50.0
9-methylfluorene	1	0.0	51.1	50.0
9-octadecynoic acid	1	14.0	172.0	153.3
a-(trifluoromethoxy)-a,a-difluoromethyl acetate	1	2.5	50.8	68.5
a,a'-dibromo-m-xylene	1	1.5	67.6	61.1
a,a'-dibromo-o-xylene	1	1.5	72.7	61.1
a,a'-dichloro-m-xylene	1	1.5	63.5	61.1
a,a'-dichloro-o-xylene	1	1.5	64.8	61.1
a,a'-dichloro-p-xylene	1	1.5	64.2	61.1
a-alanyl-a-alanine (DL)	1	3.0	68.7	72.1
acenaphthene	2	0.0	58.5	44.3

acenaphthylene	2	0.0	42.4	44.3
acetaldehyde	1	0.0	22.5	50.0
acetamide	1	0.0	44.2	50.0
acetanilide	1	1.0	55.9	57.4
acetone	2	0.0	32.4	44.3
acetonitile	1	0.0	39.5	50.0
acetylacetone enol	1	0.0	56.9	50.0
acetylene	2	0.0	37.3	44.3
a-chloroacetic acid	1	0.5	42.2	53.7
a-chloroacetic acid	1	0.5	48.8	53.7
acridine	2	0.0	48.5	44.3
acrylamide	1	0.0	42.8	50.0
acrylic acid	2	0.0	39.1	44.3
acrylonitrile	1	0.0	39.1	50.0
a-D-glucopyranose (a-D-glucose)	1	3.0	81.0	72.1
a-D-glucose	1	3.0	75.9	72.1
adipic acid	1	4.0	81.7	79.5
alanylglycine (with decomp)	1	3.0	111.4	72.1
allobarbitiol	1	2.5	73.0	68.5
a-methylacrylic acid	1	0.0	28.0	50.0
a-methylstyrene	1	0.0	47.5	50.0
a-naphthol	1	0.0	62.4	50.0
a-naphthyl acetate	1	1.0	63.3	57.4
androstanolone	1	0.0	59.6	50.0
aniline	2	0.0	39.5	44.3
anisaldazine	1	2.0	67.3	64.8
anthracene	4	0.0	60.1	38.5
anthraquinone	4	0.0	58.4	38.5
azelaic acid	1	7.0	86.0	101.7
azoxybenzene	1	1.5	58.0	61.1
azulene	2	0.0	46.9	44.3
b(4-chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	1	4.0	64.8	79.5
b-alanyl-b-alanine	1	3.0	121.4	72.1
barbital	1	1.5	54.0	61.1
benzaldehyde	2	0.0	43.2	44.3
benzamide	1	0.0	46.0	50.0
benzanilide	1	1.0	67.8	57.4
benzene	12	0.0	35.4	29.4
benzene-hexa-n-hexanoate	1	30.0	281.7	271.5
benzidine	4	0.0	47.7	38.5
benzil	1	0.0	64.5	50.0
benzimidazole	2	0.0	43.4	44.3
benzo[c]cinnoline	2	0.0	48.4	44.3
benzofluoranthene	1	0.0	43.6	50.0
benzoic acid	2	0.0	45.5	44.3
benzoic anhydride	1	1.0	54.8	57.4
benzonitrile	2	0.0	42.2	44.3
benzophenone	2	0.0	56.7	44.3
benzothiazole	1	0.0	46.4	50.0
benzothiophene	1	0.0	38.9	50.0
benzotrichloride	1	0.0	59.1	50.0
benzotrifluoride	1	0.0	56.4	50.0

benzoxazole	1	0.0	55.5	50.0
benzyl alcohol	1	0.5	34.1	53.7
benzyl benzoate	1	2.0	69.7	64.8
benzylbromide	1	0.5	48.6	53.7
benzyliodide	1	0.5	44.1	53.7
benzylmethylsulfone	1	0.5	63.7	53.7
biphenyl	4	0.0	54.6	38.5
bis(2-cyanoethyl)-N-nitroamine	1	4.0	137.6	79.5
bis-(4-aminophenyl)methane	1	1.0	25.4	57.4
bis(4-chlorophenyl)acetic acid	1	1.0	71.9	57.4
bis-[3,5-di-tert-butyl-4-hydroxybenzyl]sulfide	1	7.0	103.3	101.7
bis-hydroxyethylpiperazine	1	6.0	64.0	94.3
bromobenzene	2	0.0	44.1	44.3
bromocyclohexane	1	3.0	49.7	72.1
bromomethane	1	0.0	33.3	50.0
bromotrichloromethane	3	0.0	28.7	40.9
butanal	1	1.5	62.7	61.1
butane	1	1.0	53.6	57.4
butanoic acid	1	1.5	41.8	61.1
butyl 4-aminobenzoate	1	4.0	61.8	79.5
butyl 9-hydroxy-9H-fluorene-9-carboxylate	1	4.0	74.3	79.5
butyl acrylate	1	4.0	82.6	79.5
butyl alcohol	1	2.0	50.5	64.8
butyl butanoate	1	5.5	82.2	90.6
butyl ethyl sulfide	1	4.0	69.6	79.5
butyl octadecanoate	1	20.0	132.8	197.6
caffeine	1	0.0	47.6	50.0
carbazole	2	0.0	52.2	44.3
carbon tetrabromide	12	0.0	29.5	29.4
carbon tetrachloride	12	0.0	31.3	29.4
carbon tetrafluoride	12	0.0	27.0	29.4
chlorobenzene	2	0.0	41.9	44.3
chlorocyclohexane	1	3.0	45.7	72.1
chlorocyclopentane	1	2.0	48.6	64.8
chlorodifluoromethane	1	0.0	36.2	50.0
chloroethane	1	0.0	33.0	50.0
chloroethyl methacrylate	1	3.0	72.3	72.1
chloropentafluorobenzene	2	0.0	55.5	44.3
chlorotrifluoroethylene	1	0.0	48.3	50.0
cholesterol*	1	4.0	73.4	79.5
chroman	1	1.0	60.3	57.4
chromone	1	0.0	52.4	50.0
chrysene	2	0.0	55.3	44.3
cinnamic acid	1	1.0	55.7	57.4
cinnamic anhydride	1	3.0	102.0	72.1
cinnamyl alcohol	1	1.5	51.0	61.1
cis,cis-1,3,5-tri-tert-butylcyclohexane	1	2.0	68.1	64.8
cis,trans-1,3,5-tri-tert-butylcyclohexane	1	2.0	53.2	64.8
cis-1,2-cyclohexanediol	1	3.0	64.1	72.1
cis-1,2-dimethylcyclohexane	1	3.0	55.2	72.1
cis-1,2-dimethylcyclopentane	1	2.0	54.6	64.8
cis-1,3-dimethylcyclohexane	1	3.0	54.8	72.1
cis-1,4-dimethylcyclohexane	1	3.0	50.0	72.1

cis-1,4-di-tert-butylcyclohexane	1	4.0	30.0	79.5
cis-2-butene	2	0.0	54.4	44.3
cis-2-hexene	1	2.0	67.3	64.8
cis-2-pentene	1	1.0	58.4	57.4
cis-3-chloro-2-butenoic acid	1	0.5	41.4	53.7
cis-6-octadecenoic acid	1	14.0	156.4	153.3
cis-9-octadecenoic acid	1	14.0	138.2	153.3
cis-crotonic acid	1	0.5	36.5	53.7
coronene	12	0.0	27.0	29.4
cortisone	1	0.5	74.5	53.7
cortisone acetate	1	2.0	75.5	64.8
coumarin	1	0.0	55.9	50.0
cyanamide	10	0.0	27.6	30.9
cyanoacetamide	1	0.5	59.1	53.7
cyanocyclohexane	1	3.0	47.3	72.1
cyanogen	2	0.0	33.1	44.3
cyclobutane	2	0.0	45.1	44.3
cycloheptane	1	4.0	47.6	79.5
cycloheptanol	1	4.0	28.5	79.5
cycloheptatriene	1	1.0	17.7	57.4
cycloheptene	1	3.0	42.1	72.1
cyclohexane	1	3.0	45.8	72.1
cyclohexanethiol	1	3.0	52.7	72.1
cyclohexanol	1	3.0	39.3	72.1
cyclohexanone	1	2.5	44.6	68.5
cyclohexanone oxime	1	2.0	35.4	64.8
cyclohexene	1	2.0	49.9	64.8
cyclohexylbenzene	1	2.5	54.5	68.5
cycloocta-1,5-diene	1	3.0	48.2	72.1
cyclooctane	1	5.0	48.9	86.9
cyclooctanol	1	5.0	15.1	86.9
cyclooctatetraene	4	0.0	41.9	38.5
cyclooctene	1	4.0	58.5	79.5
cyclopentadiene	2	0.0	45.4	44.3
cyclopentane	1	2.0	46.0	64.8
cyclopentanethiol	1	2.0	50.4	64.8
cyclopentanol	1	2.0	24.3	64.8
cyclopentene	1	1.0	29.8	57.4
cyclopentyl methyl sulfide	1	2.5	59.4	68.5
cyclopentylamine	1	2.0	46.2	64.8
cyclopropane	6	0.0	37.4	35.1
cyclopropylamine	2	0.0	55.4	44.3
D mannitol	1	5.0	127.8	86.9
D sorbitol	1	5.0	82.4	86.9
decachlorobiphenyl	4	0.0	68.1	38.5
decacyclene	1	0.0	38.1	50.0
decanal	1	7.5	114.1	105.4
decanoic acid	1	7.5	91.4	105.4
decyl methacrylate	1	9.0	121.9	116.4
deoxycorticosterone	1	0.5	67.6	53.7
deoxycorticosterone acetate	1	2.0	69.0	64.8
dexamethasone	1	0.5	78.0	53.7
diaminoethane	1	1.0	81.2	57.4

dibenzo[c,e][1,2]dithiin	2	0.0	50.0	44.3
dibenzodioxin	4	0.0	58.6	38.5
dibenzofuran	2	0.0	52.3	44.3
dibenzothiophene	2	0.0	58.2	44.3
dibromodichloromethane	2	0.0	28.8	44.3
dibromodifluoroethylene	2	0.0	43.2	44.3
dichloroacetic acid	1	0.0	43.1	50.0
dichloromethane	1	0.0	34.6	50.0
dicyanomethane	1	0.0	35.4	50.0
diethyl disulfide	1	3.0	54.8	72.1
diethyl ether	1	2.0	45.8	64.8
diethyl o-phthalate	1	4.5	66.7	83.2
diethyl sulfide	1	2.0	70.4	64.8
diethyl terephthalate	1	4.5	77.8	83.2
diethylstilbestrol	1	3.0	71.6	72.1
difluoromethane	1	0.0	32.0	50.0
dihydroxyethane	1	1.0	38.2	57.4
diiodomethane	1	0.0	43.2	50.0
diisopropyl ketone	1	1.5	54.7	61.1
diisopropyl sulfide	1	2.0	53.4	64.8
dimethoxymethane	1	2.0	49.6	64.8
dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	1	2.0	65.1	64.8
dimethyl amine	1	0.0	29.7	50.0
dimethyl ether	1	0.0	37.5	50.0
dimethyl fumarate	1	3.0	93.7	72.1
dimethyl maleate	1	3.0	57.6	72.1
dimethyl oxalate	1	2.0	64.3	64.8
dimethyl sulfide	1	0.0	45.6	50.0
dimethyl sulfoxide	2	0.0	49.3	44.3
dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	1	2.5	70.0	68.5
dimethylaminoethyl methacrylate	1	4.0	70.9	79.5
dimethyldisulfide	1	1.0	48.8	57.4
dimethylsulfone	2	0.0	47.9	44.3
di-n-butyl succinate	1	10.0	119.7	123.8
di-n-butyl sulfide	1	6.0	93.9	94.3
diphenyl ether	1	1.0	57.4	57.4
diphenyl sulfone	1	0.0	54.7	50.0
diphenylacetic acid	1	1.0	74.3	57.4
diphenylacetylene	4	0.0	61.4	38.5
diphenylamine	1	1.0	54.8	57.4
diphenylcarbinol	1	1.0	67.9	57.4
diphenylmethane	1	1.0	62.3	57.4
diphenylsulfide	1	1.0	54.2	57.4
dipropyl disulfide	1	5.0	73.6	86.9
dipropyl sulfide	1	4.0	71.2	79.5
DL 3,6-dimethyl-1,4-dioxane-2,5-dione	2	0.0	62.1	44.3
DL lactic acid	1	0.5	39.1	53.7
d-limonene	1	1.5	57.1	61.1
dodecane	1	9.0	139.7	116.4
dodecanedioic acid	1	10.0	125.6	123.8
dodecanoic acid	1	9.5	115.7	120.1
dodecanol	1	10.0	133.8	123.8
dotriacontane	1	30.0	345.1	271.5

dulcitol	1	5.0	141.4	86.9
d-valerolactone	1	2.5	42.9	68.5
E-3-chloro-2-butenoic acid	1	0.5	41.4	53.7
e-caprolactam	1	3.5	46.9	75.8
e-caprolactone	1	3.5	50.8	75.8
eicosanoic acid	1	18.0	198.7	182.9
estrone	1	0.0	90.1	50.0
ethane	20	0.0	31.2	25.2
ethanethioamide	1	0.0	47.6	50.0
ethanoic acid	2	0.0	39.2	44.3
ethanol	1	0.0	57.4	50.0
ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	1	5.0	83.1	86.9
ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	1	3.0	75.6	72.1
ethyl 4-aminobenzoate	1	2.0	64.9	64.8
ethyl acetate	1	1.5	55.4	61.1
ethyl carbamate	1	1.5	47.3	61.1
ethyl cyanoacetate	1	2.5	47.7	68.5
ethyl docosanoate	1	22.0	90.4	212.4
ethyl eicosanoate	1	20.0	69.3	197.6
ethyl hexaconsanate	1	26.0	124.8	241.9
ethyl hexadecanoate	1	16.0	50.9	168.1
ethyl mercaptan	1	0.0	25.4	50.0
ethyl methyl sulfide	1	1.0	58.4	57.4
ethyl N-benzoyl-n-(3,4-dichlorophenyl)-dl-alaninate	1	4.0	79.2	79.5
ethyl nitrate	1	0.0	47.8	50.0
ethyl phenyl carbamate	1	2.0	49.9	64.8
ethyl propyl ether	1	3.0	57.6	72.1
ethyl propyl sulfide	1	3.0	67.8	72.1
ethyl tetracosanate	1	28.0	105.3	256.7
ethyl triacontanoate	1	30.0	154.0	271.5
ethyl(1,1-dimethylpropyl)malononitrile	1	3.0	62.6	72.1
ethylbenzene	1	0.5	51.4	53.7
ethylcyclohexane	1	3.5	51.6	75.8
ethylcyclopentane	1	2.5	50.9	68.5
ethylene	4	0.0	32.2	38.5
ethylene carbonate	1	1.5	43.0	61.1
ethylene oxalate	1	2.0	32.3	64.8
ethylene oxide	2	0.0	32.2	44.3
ethylmethylsulfone	1	0.0	36.7	50.0
fluorene	2	0.0	50.5	44.3
fluorobenzene	2	0.0	49.0	44.3
fluorotrichloromethane	3	0.0	42.4	40.9
furan	2	0.0	33.9	44.3
furfural	1	0.0	61.1	50.0
furfuryl alcohol	1	0.5	50.7	53.7
glutaric acid	1	3.0	63.0	72.1
glyceryl triacetate	1	6.5	93.7	98.0
glyceryl trilaurate	1	36.0	386.6	315.8
glyceryl trimyristate	1	42.0	460.9	360.0
glyceryl tripalmitate	1	48.0	529.3	404.3
glyceryl tristearate	1	54.0	588.0	448.6
heptadecanoic acid	1	15.0	176.2	160.7
heptanal	1	4.5	99.8	83.2

heptane	1	4.0	76.9	79.5
heptanoic acid	1	4.5	67.2	83.2
hexachlorobenzene	12	0.0	47.2	29.4
hexachlorocyclopropane	6	0.0	49.5	35.1
hexachloroethane	6	0.0	53.2	35.1
hexacontane	1	58.0	500.4	478.2
hexadecane	1	14.0	176.8	153.3
hexadecanoic acid	1	14.0	163.3	153.3
hexafluoroacetone	1	0.0	56.7	50.0
hexafluorobenzene	12	0.0	41.6	29.4
hexafluoroethane	20	0.0	51.4	25.2
hexamethylbenzene	12	0.0	51.0	29.4
hexanal	1	3.5	63.3	75.8
hexanamide	1	3.5	67.1	75.8
hexatriacontane	1	34.0	371.1	301.0
hexyl ethanoate	1	5.5	93.5	90.6
hexyl N-phenylcarbamate	1	6.0	99.9	94.3
hydrazobenzene (1,2-diphenylhydrazine)	1	2.0	43.3	64.8
hydrocinnamic acid	1	2.0	55.0	64.8
hydrocortisone	1	0.5	73.7	53.7
hydrocortisone-21-acetate	1	2.0	74.5	64.8
imidazole	1	0.0	35.4	50.0
indene	1	0.0	37.5	50.0
iodobenzene	2	0.0	40.3	44.3
iodomethane	3	0.0	44.1	40.9
isobutane	3	0.0	40.1	40.9
isobutene	2	0.0	44.7	44.3
isobutyl alcohol	1	1.0	36.9	57.4
isobutyl mercaptan	1	1.0	38.8	57.4
isochroman	1	1.0	60.4	57.4
isonicotinic acid	2	0.0	54.2	44.3
isopropyl 4,4'-dibromobenzilate	1	3.0	70.5	72.1
isopropyl ether	1	2.0	64.2	64.8
isopropyl methyl ketone	1	0.5	51.9	53.7
isopropyl methyl sulfide	1	1.0	54.5	57.4
isopropyl nitrate	1	0.0	52.9	50.0
isopropyl phenylcarbamate	1	3.0	53.9	72.1
isopropyl-3-chlorophenylcarbamate	1	3.0	56.5	72.1
isopropylbenzene	1	0.5	41.3	53.7
isoquinoline	1	0.0	45.2	50.0
L-carvone	1	0.0	46.6	50.0
levulinic acid	1	2.0	30.1	64.8
L-iditol	1	5.0	87.6	86.9
linoelaidic acid	1	12.0	157.4	138.6
maleic anhydride	2	0.0	37.6	44.3
malonamide	1	1.0	85.1	57.4
m-aminophenol	1	0.0	57.6	50.0
m-bromophenol	1	0.0	49.3	50.0
methacrylamide	1	0.0	39.0	50.0
methanethiol	3	0.0	40.9	40.9
methanol	10	0.0	21.5	30.9
methoxybenzene	1	0.5	48.0	53.7
methyl 2-(2,4,5-trichlorophenoxy)acetate	1	3.0	84.2	72.1

methyl 2-(2,4,5-trichlorophenoxy)butyrate	1	4.0	91.2	79.5
methyl 2-(2,4,5-trichlorophenoxy)propionate	1	3.0	88.6	72.1
methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	1	4.0	86.1	79.5
methyl 2,4-dichlorophenoxyacetate	1	3.0	79.6	72.1
methyl 3,6-dichloro-2-methoxybenzoate	1	2.0	60.7	64.8
methyl 3-m-tolylcarbamoyloxyphenylcarbamate	1	4.0	93.5	79.5
methyl 4-(2,4-dichlorophenoxy)butyrate	1	5.0	105.4	86.9
methyl 4-amino-3,5,6-trichloro-2-picolinate	1	1.0	67.9	57.4
methyl 4-aminobenzoate	1	1.0	58.6	57.4
methyl 4-hydroxybenzoate	1	1.0	61.0	57.4
methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	1	3.0	73.4	72.1
methyl acetate	1	0.5	42.8	53.7
methyl acrylate	1	1.0	49.3	57.4
methyl a-D-mannopyranoside	1	4.0	98.2	79.5
methyl benzoate	1	1.0	53.3	57.4
methyl butyl sulfide	1	3.0	70.9	72.1
methyl carbamate	1	0.5	50.8	53.7
methyl chloride	10	0.0	36.8	30.9
methyl docosanoate	1	21.0	89.9	205.0
methyl isopropyl ether	1	1.0	46.0	57.4
methyl methacrylate	1	1.0	54.4	57.4
methyl myristate	1	13.0	172.2	146.0
methyl n-butyl ether	1	3.0	68.9	72.1
methyl n-decyl ether	1	9.0	130.2	116.4
methyl nitrate	1	0.0	43.3	50.0
methyl N-phenylcarbamate	1	2.0	44.8	64.8
methyl octadecanoate	1	17.0	61.9	175.5
methyl palmitate	1	15.0	221.8	160.7
methyl perfluorobutanoate	1	2.5	61.5	68.5
methyl p-N,N-dimethylaminobenzoate	1	2.0	70.1	64.8
methyl propyl ether	1	2.0	57.2	64.8
methyl propyl sulfide	1	2.0	61.9	64.8
methyl tert-butyl ether	1	0.0	46.2	50.0
methyl tert-butyl sulfide	1	0.0	44.1	50.0
methyl tetrachloroterephthalic acid ester	1	1.5	38.0	61.1
methyl-3,4-dichlorophenylcarbamate	1	2.0	60.8	64.8
methylamine	10	0.0	34.1	30.9
methylcyclobutane	1	1.0	41.6	57.4
methylcyclohexane	1	3.0	45.6	72.1
methylcyclopentane	1	2.0	53.0	64.8
methylenecyclobutane	1	0.5	42.3	53.7
methylhydrazine	1	0.0	47.2	50.0
methylphenylsulfide	1	0.5	57.9	53.7
methylphosphonyl chlorofluoride	1	0.0	47.3	50.0
methylphosphonyl dichloride	2	0.0	59.1	44.3
methylphosphonyl difluoride	2	0.0	50.3	44.3
m-hydroxytoluene	1	0.0	37.5	50.0
m-nitrobenzoic acid	1	0.0	46.7	50.0
m-nitrophenol	1	0.0	51.7	50.0
mono(2,2-dimethylhydrazide) butanedioic acid	1	4.0	85.7	79.5
m-phenylenediamine	2	0.0	45.9	44.3
m-terphenyl	2	0.0	62.8	44.3
m-toluic acid	1	0.0	41.2	50.0

m-toluidine	1	0.0	36.4	50.0
m-xylene	2	0.0	51.4	44.3
myo-inositol	1	3.0	96.4	72.1
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	1	6.0	76.9	94.3
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl) benzeneamine	1	4.5	72.5	83.2
N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	1	2.5	78.3	68.5
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	1	1.5	81.0	61.1
N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea	1	3.0	68.8	72.1
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	1	4.0	46.3	79.5
N-(4-chlorophenyl)-2,2-dimethylpentanamide	1	4.0	64.7	79.5
N'-(4-chlorophenyl)-N-methoxy-N-methylurea	1	3.0	63.8	72.1
N-(cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl)benzenamine	1	7.0	73.6	101.7
N,N'-(2-hydroxyethyl)-1,4-diaminoanthraquinone	1	6.0	62.0	94.3
N,N-(2-hydroxyethyl)-4-(4-nitrophenyl)azoaniline	1	6.0	67.0	94.3
N,N-(2-hydroxyethyl)-4-phenylazoaniline	1	5.0	73.6	86.9
N,N-diethyl-2-(1-naphthyloxy)propionamide	1	5.0	71.2	86.9
N,N-dimethyl-1,3-propanediamine	1	3.0	63.7	72.1
N,N-dimethyl-2,2-diphenylacetamide	1	2.0	62.5	64.8
N,N-dimethyl-2,2-diphenylbenzeneacetamide	1	2.0	63.3	64.8
N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide	1	5.0	81.1	86.9
N,N-dimethyl-4-phenylazoaniline	1	1.0	59.3	57.4
N,N-dimethylaniline	1	0.5	46.3	53.7
N,N-dimethylformamide	1	0.5	42.0	53.7
N,N'-dimethylhydrazine	1	1.0	51.6	57.4
N,N-dimethylhydrazine	1	0.0	46.6	50.0
N,N'-dimethyl-N,N'dinitro-1,2-ethanediamine	1	3.0	147.1	72.1
N,N'-dimethyl-N,N'dinitro-1,6-hexanediamine	1	7.0	186.3	101.7
N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea	1	2.0	68.7	64.8
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea	1	3.0	78.7	72.1
N,N'-di-n-hexyladipamide	1	16.0	94.6	168.1
N,N'-dinitro-diaminomethane	1	2.0	96.6	64.8
N,N'-dinitroethanediamine	1	3.0	65.6	72.1
N,N'-di-n-propyladipamide	1	10.0	79.9	123.8
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	1	2.0	99.8	64.8
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-propanamide	1	6.0	64.4	94.3
N-[4-methyl-3-[[(trifluoromethyl)sulfonyl]amino]phenyl] acetamide	1	2.0	88.8	64.8
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea	1	2.0	67.7	64.8
N-acetyl-D-leucine amide	1	4.0	50.0	79.5
N-acetylglycine amide	1	2.0	62.7	64.8
N-acetylglycyl-L-prolinamide	1	4.5	71.2	83.2
N-acetyl-L-alanine amide	1	2.0	50.3	64.8
N-acetyl-L-isoleucinamide	1	4.0	78.9	79.5
N-acetyl-L-prolyl-glycinamide	1	4.5	74.2	83.2

N-acetyl-pyrazinamide	1	1.5	64.4	61.1
N-acetylsarcosinamide	1	2.0	66.4	64.8
N-allyl-N-phenylthiourea	1	3.5	73.6	75.8
naphthalene	4	0.0	54.0	38.5
naphthalene 1,8-disulfide	2	0.0	32.9	44.3
naphthalene 1,8-disulfide s-oxide	1	0.0	55.3	50.0
N-benzylaniline	1	2.0	54.8	64.8
N-butyl dodecanamide	1	14.0	121.1	153.3
n-butyl mercaptan	1	2.0	66.4	64.8
N-butyl tetradecanamide	1	16.0	133.9	168.1
n-butylbenzene	1	2.5	60.6	68.5
n-butylcyclohexane	1	5.5	71.3	90.6
n-butylcyclopentane	1	4.5	68.5	83.2
N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea	1	5.0	72.7	86.9
N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline	1	8.0	107.8	109.1
N-butylurea	1	3.5	64.4	75.8
n-decane	1	7.0	117.9	101.7
N-decyl hexadecanamide	1	24.0	196.6	227.2
n-decyl-a-cyanoacrylate	1	10.0	141.9	123.8
N-decylundecanamide	1	19.0	123.6	190.3
N-dimethylaminosuccinamic acid	1	4.0	85.7	79.5
n-docosane	1	20.0	245.0	197.6
n-dodecylcyclohexane	1	13.0	177.1	146.0
n-dononacontahectane	1	190.0	1751.2	1452.6
n-eicosane	1	18.0	219.6	182.9
neopentyl-4,4,4-trinitrobutyrate	1	4.5	67.7	83.2
n-ethyl-a-cyanoacrylate	1	2.0	52.9	64.8
N-ethylurea	1	1.5	39.4	61.1
n-hectane	1	98.0	1004.0	773.4
n-heneicosane	1	19.0	202.7	190.3
n-heptacosane	1	25.0	265.7	234.6
n-heptadecane	1	15.0	174.7	160.7
N-heptylmyristamide	1	19.0	163.6	190.3
n-hexacosane	1	24.0	289.3	227.2
n-hexane	1	3.0	73.6	72.1
N-hexyl decanamide	1	14.0	119.6	153.3
N-hexyl hexadecanamide	1	20.0	166.1	197.6
N-hexyl tetradecanamide	1	18.0	151.9	182.9
nicotinic acid	1	0.0	53.9	50.0
N-isopropylcarbazole	1	1.0	47.4	57.4
N-isopropylurea	1	1.5	52.0	61.1
nitrobenzene	2	0.0	43.5	44.3
nitroethane	1	0.0	53.6	50.0
nitromethane	2	0.0	39.6	44.3
N-laurylnonanamide	1	19.0	196.7	190.3
N-methyl O-methyl O-2-chloro-4-tert-butylphenyl phosphoramidate	1	2.5	66.2	68.5
N-methyl-2,4,6,N-tetranitroaniline	1	0.5	64.2	53.7
N-methyl-2-chlorophenylcarbamic acid ester	1	2.0	60.1	64.8
N-methylacetamide	1	0.5	32.0	53.7
N-methylcarbazole	2	0.0	47.3	44.3

N-methyldiphenylacetamide	1	2.0	68.7	64.8
N-methyl-N-nitrobutanamine	1	3.0	113.5	72.1
N-methylpyrrole	2	0.0	36.1	44.3
N-methylurea	1	0.5	37.2	53.7
N-myristylheptanamide	1	19.0	164.4	190.3
N-nitro-bis(N,N-cyanomethyl) amine	1	2.0	105.3	64.8
N-nitro-N-methylaminomethane	1	0.0	115.2	50.0
n-nonacosane	1	27.0	286.1	249.3
n-octacosane	1	26.0	300.3	241.9
n-octane	1	5.0	95.8	86.9
n-octylbenzene	1	7.0	127.9	101.7
nonadecane	1	17.0	201.4	175.5
nonadecanoic acid	1	17.0	195.9	175.5
nonanal	1	6.5	116.6	98.0
nonane	1	6.0	99.0	94.3
nonanoic acid	1	6.5	92.1	98.0
nonyl acrylate	1	9.0	98.8	116.4
nonyl phenylcarbamate	1	10.0	85.8	123.8
N-palmitoyl-pyrazinamide	1	15.0	142.9	160.7
n-pentacontane	1	48.0	504.2	404.3
n-pentacosane	1	23.0	258.2	219.8
n-pentadecane	1	13.0	156.0	146.0
n-pentatriacontane	1	33.0	368.0	293.6
N-phenyl-N[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)	1	4.0	63.0	79.5
n-propylbenzene	1	1.5	53.4	61.1
n-propylcyclohexane	1	4.5	58.2	83.2
N-propylstearamide	1	19.0	187.4	190.3
N-propylurea	1	2.5	38.4	68.5
N-salicylidene-m-aminobenzoic acid	1	0.0	71.4	50.0
N-stearylpropanamide	1	19.0	165.6	190.3
N-tert-butylurea	1	0.5	73.9	53.7
n-tetracosane	1	22.0	266.8	212.4
n-tetratetracontane	1	42.0	403.1	360.0
n-tricosane	1	21.0	237.7	205.0
n-tridecane	1	11.0	136.3	131.2
n-undecane	1	8.0	118.6	109.1
N-vinylpyrrolidone	1	1.0	53.4	57.4
O-(2,4-dichlorophenyl) O-methyl-(1-methylethyl) phosphoramidothioate	1	3.5	91.2	75.8
O-(2-chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate	1	2.5	89.8	68.5
O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate	1	2.5	95.8	68.5
O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphonothioate	1	2.0	90.7	64.8
O,O,O',O'-tetramethyl O,O'-thiodi-p-phenylene bis(phosphorothioate)	1	7.0	108.9	101.7
O,O-diethyl O-4-nitrophenyl phosphorothioate	1	4.5	56.5	83.2
O,O-diethyl O-quinoxalin-2-yl phosphothioate	1	4.5	83.5	83.2
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl) phosphate	1	4.5	50.0	83.2

O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl) phosphorothioate	1	4.5	77.9	83.2
O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	1	8.0	98.6	109.1
O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	1	2.5	60.5	68.5
O,O-dimethyl O-(4-aminosulfonylphenyl) phosphorothioate	1	2.5	76.1	68.5
O,O-dimethyl O-4-nitrophenyl phosphorothioate	1	2.5	65.1	68.5
O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate	1	4.5	63.8	83.2
O,O-dimethyl S-phthalimidomethyl phosphorodithioate	1	3.5	78.6	75.8
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl) phosphorothioate	1	2.5	81.3	68.5
O,S-dimethyl phosphoroamidothioate	1	1.0	42.1	57.4
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a] pyrimidin-2-yl O,O-diethyl phosphorothioate	1	7.0	84.2	101.7
o-aminophenol	1	0.0	76.0	50.0
octadecanamide	1	16.0	158.8	168.1
octadecane	1	16.0	204.6	168.1
octadecanoic acid	1	16.0	178.7	168.1
octadecanol	1	17.0	209.7	175.5
octafluoropropane	1	0.0	39.6	50.0
octafluorotetrahydrothiophene	2	0.0	82.4	44.3
octanal	1	5.5	89.7	90.6
octanoic acid	1	5.5	73.8	90.6
octyl methacrylate	1	7.5	104.6	105.4
O-ethyl O-(4-nitrophenyl)phenylphosphonothioate	1	4.0	81.3	79.5
o-hydroxyacetanilide	1	1.0	58.3	57.4
o-hydroxybiphenyl	1	0.0	48.1	50.0
o-hydroxytoluene	1	0.0	52.0	50.0
o-nitrobenzoic acid	1	0.0	66.8	50.0
o-nitrophenol	1	0.0	54.8	50.0
o-phenylenediamine	2	0.0	61.8	44.3
o-phenylenepyrene	1	0.0	49.4	50.0
o-terphenyl	1	0.5	52.2	53.7
o-toluic acid	1	0.0	53.5	50.0
o-toluidine	1	0.0	32.4	50.0
o-xylene	2	0.0	54.9	44.3
p,p'-dichlorobenzophenone	2	0.0	71.7	44.3
p-a-cumylphenol	1	1.0	62.6	57.4
p-aminobenzene sulphonamide	1	0.0	58.4	50.0
p-aminophenol	2	0.0	56.2	44.3
p-benzoquinone	4	0.0	47.6	38.5
p-bromotoluene	2	0.0	50.1	44.3
p-chlorobenzyl p-chlorophenyl sulfide	1	2.0	93.7	64.8
p-chlorotoluene	2	0.0	48.3	44.3
p-dioxanone	1	2.5	53.5	68.5
pentabromophenol	2	0.0	63.7	44.3
pentachloroaniline	2	0.0	37.0	44.3
pentachlorobenzene	2	0.0	57.6	44.3

pentachloronitrobenzene	1	0.0	44.0	50.0
pentachlorophenol	2	0.0	37.1	44.3
pentadecanoic acid	1	13.0	153.0	146.0
pentaerythritol	1	3.0	108.8	72.1
pentaerythritol tetrafluoride	1	4.0	67.1	79.5
pentaerythrityl tetrabromide	1	4.0	64.5	79.5
pentafluoroaniline	2	0.0	59.4	44.3
pentafluorobenzene	2	0.0	48.2	44.3
pentafluorochloroethane	1	0.0	43.6	50.0
pentafluoroethane	1	0.0	13.0	50.0
pentafluoronitrobenzene	1	0.0	47.1	50.0
pentafluorophenol	2	0.0	56.6	44.3
pentamethylbenzene	2	0.0	39.3	44.3
pentane	1	2.0	58.5	64.8
pentanoic acid	1	2.5	59.1	68.5
pentyl 4-aminobenzoate	1	5.0	73.6	86.9
perfluorotoluene	1	0.0	55.5	50.0
perylene	4	0.0	57.9	38.5
p-ethoxyacetanilide	1	3.0	76.7	72.1
phenanthrene	2	0.0	44.8	44.3
phenanthridine	1	0.0	60.2	50.0
phenazine	4	0.0	46.5	38.5
phenol	2	0.0	36.7	44.3
phenolphthalein	1	0.5	95.6	53.7
phenoxathiin	2	0.0	61.6	44.3
phenyl glycidyl ether	1	2.0	61.9	64.8
phenyl vinyl sulfone	1	0.0	34.1	50.0
phenylacetic acid	1	1.0	41.4	57.4
phenylacetylene	2	0.0	41.5	44.3
phenylaminoethyl methacrylate	1	4.5	85.6	83.2
phenylhydrazine	1	0.5	56.1	53.7
phenyl-o-tolylmethane	1	1.0	68.8	57.4
phenylurea	1	1.0	56.3	57.4
phthalazine	2	0.0	36.5	44.3
phthalic anhydride	2	0.0	57.3	44.3
p-hydroxyacetanilide	1	1.0	59.0	57.4
p-hydroxytoluene	2	0.0	41.3	44.3
picene	2	0.0	55.2	44.3
picolinic acid	1	0.0	73.0	50.0
picric acid	1	0.0	43.4	50.0
pimilic acid	1	5.0	73.2	86.9
p-iodotoluene	2	0.0	48.8	44.3
piperidine	1	3.0	56.7	72.1
pivaldehyde	1	0.0	38.6	50.0
p-methacryloyloxybenzoic acid	1	2.0	74.7	64.8
p-methoxyacetanilide	1	2.0	69.5	64.8
p-n-hexyloxybenzylideneaniline	1	6.0	98.7	94.3
p-nitrobenzoic acid	2	0.0	72.0	44.3
p-nitrophenol	2	0.0	47.0	44.3
p-phenylazoaniline	2	0.0	54.5	44.3
p-phenylenediamine	4	0.0	52.6	38.5

p-quaterphenyl	4	0.0	66.2	38.5
prednisolone	1	0.5	75.8	53.7
pregnenolone acetate	1	1.0	64.8	57.4
progesterone	1	0.0	66.8	50.0
propanal	1	0.5	50.1	53.7
propane	1	0.0	41.2	50.0
propene	1	0.0	33.2	50.0
propionic acid	1	0.5	42.2	53.7
propionitrile	1	0.0	37.6	50.0
propyl 4-aminobenzoate	1	3.0	59.2	72.1
propyl 4-hydroxybenzoate	1	3.0	75.8	72.1
propyl N-phenyl carbamate	1	4.0	63.7	79.5
propylcyclopentane	1	3.5	64.4	75.8
propylene carbonate	1	1.5	44.1	61.1
propylene oxide	1	0.0	40.7	50.0
p-terphenyl	4	0.0	77.0	38.5
p-toluic acid	2	0.0	50.2	44.3
p-toluidine	2	0.0	56.5	44.3
p-xylene	4	0.0	59.8	38.5
pyrazine	4	0.0	39.5	38.5
pyrazole	1	0.0	41.4	50.0
pyrene	4	0.0	43.4	38.5
pyridine	2	0.0	35.8	44.3
pyromellitic dianhydride 1,2,5,6-benzenetetracarboxylic dianhydride	4	0.0	28.4	38.5
pyrrole	2	0.0	31.7	44.3
pyrrolidine	1	2.0	42.4	64.8
quinazoline	1	0.0	52.8	50.0
quinoline	1	0.0	41.5	50.0
quinoxaline	2	0.0	38.6	44.3
S-(+)-4-isobutyl-a-methylphenyl acetic acid	1	3.0	57.5	72.1
S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate	1	5.5	78.3	90.6
S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethyl phoshorodithioate	1	3.5	80.4	75.8
S-2,3,3-trichloroallyl diisopropylthiocarbamate	1	5.5	88.5	90.6
S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl-O,O-dimethyl phosphorodithioate	1	4.5	90.6	83.2
sebacic acid	1	8.0	101.0	109.1
spiropentane	4	0.0	38.7	38.5
ß,ß-binaphthyl	2	0.0	84.3	44.3
ß-chloroacetic acid	1	0.5	36.7	53.7
ß-chloroacetic acid	1	0.5	42.3	53.7
ß-naphthol	1	0.0	47.7	50.0
ß-naphthyl acetate	1	1.0	58.6	57.4
ß-propiolactone	1	0.5	39.2	53.7
ß-thiolactic acid	1	0.5	58.1	53.7
styrene	1	0.0	45.2	50.0
suberic acid	1	6.0	69.4	94.3
succinic acid	1	2.0	72.1	64.8
succinimide	2	0.0	42.5	44.3

succinonitrile	1	1.0	37.8	57.4
terephthalyl dichloride	2	0.0	65.8	44.3
tert-butyl alcohol	3	0.0	26.8	40.9
tert-butyl amine	3	0.0	35.4	40.9
tert-butyl bromide	3	0.0	39.3	40.9
tert-butyl chloride	3	0.0	45.0	40.9
tert-butyl mercaptan	3	0.0	44.9	40.9
tert-butylbenzene	1	0.0	39.1	50.0
tert-butylmethylsulfone	1	0.0	69.0	50.0
testosterone	1	0.0	68.8	50.0
testosterone acetate	1	0.5	67.5	53.7
testosterone formate	1	0.0	66.2	50.0
testosterone propionate	1	1.5	65.2	61.1
testosterone valerate	1	3.5	64.7	75.8
tetra(methylthia)methane	1	4.0	56.5	79.5
tetrachloroethene	4	0.0	47.3	38.5
tetrachloro-o-xylene	1	0.0	59.7	50.0
tetrachloro-p-xylene	4	0.0	61.4	38.5
tetracontane	1	38.0	418.4	330.5
tetracyanoethylene	4	0.0	52.8	38.5
tetradecane	1	12.0	161.5	138.6
tetradecanoic acid	1	12.0	137.9	138.6
tetrafluoroethylene	4	0.0	54.3	38.5
tetrahydrofuran	1	2.0	51.8	64.8
tetramethylsuccinonitrile	1	1.0	68.6	57.4
tetramethylurea	1	1.5	49.2	61.1
tetramethysuccinic acid	1	2.0	49.0	64.8
tetratriacontane	1	32.0	317.0	286.2
tetrazole	2	0.0	41.0	44.3
theophylline	1	0.0	51.8	50.0
thiacyclobutane	1	1.0	44.6	57.4
thiacyclohexane	1	3.0	46.2	72.1
thiacyclopentane	1	2.0	41.5	64.8
thianthrene	4	0.0	64.1	38.5
thiazole	1	0.0	40.0	50.0
thiophene	2	0.0	28.5	44.3
thiophenol	2	0.0	44.5	44.3
thiourea	2	0.0	27.8	44.3
thioxanthene 50-195	2	0.0	65.0	44.3
thioxanthone	2	0.0	72.8	44.3
thymine	1	0.0	54.5	50.0
thymol	1	0.5	67.9	53.7
toluene	2	0.0	37.1	44.3
tolyl vinyl sulfone	1	0.0	32.0	50.0
trans,cis-2,6-octadiene-1,8-dioic acid	1	4.0	59.9	79.5
trans,trans-2,6-octadiene-1,8-dioic acid	1	3.0	76.5	72.1
trans-1-(4-heptanoylphenyl)-4-heptylcyclohexane	1	14.0	70.4	153.3
trans-1,2-cyclohexanediol	1	3.0	49.7	72.1
trans-1,2-dimethylcyclohexane	1	3.0	56.8	72.1
trans-1,3-dimethylcyclohexane	1	3.0	53.9	72.1
trans-1,3-dimethylcyclopentane	1	2.0	53.1	64.8

trans-1,3-pentadiene	1	0.5	38.4	53.7
trans-1,4-dimethylcyclohexane	1	3.0	52.2	72.1
trans-1,4-di-tert-butylcyclohexane	1	4.0	47.2	79.5
trans-10-octadecenoic acid	1	14.0	179.5	153.3
trans-11-octadecenoic acid	1	14.0	184.5	153.3
trans-12-octadecenoic acid	1	14.0	174.5	153.3
trans-13-octadecenoic acid	1	14.0	174.9	153.3
trans-14-octadecenoic acid	1	14.0	174.5	153.3
trans-15-octadecenoic acid	1	14.0	178.2	153.3
trans-1-heptyl-4-(4-nonanoylphenyl)cyclohexane	1	16.0	92.6	168.1
trans-2-butene	2	0.0	58.2	44.3
trans-2-pentene	1	1.0	62.8	57.4
trans-3-octadecenoic acid	1	14.0	171.1	153.3
trans-4-octadecenoic acid	1	14.0	167.8	153.3
trans-5-octadecenoic acid	1	14.0	141.3	153.3
trans-6-octadecenoic acid	1	14.0	184.5	153.3
trans-9-octadecenoic acid (elaidic acid)	1	14.0	193.8	153.3
trans-azobenzene	4	0.0	66.1	38.5
triacontane	1	28.0	315.1	256.7
triamcinolone	1	0.5	78.4	53.7
triatriacontane	1	31.0	305.0	278.8
tribromomethane	3	0.0	39.4	40.9
trichloroacetic acid	1	0.0	17.8	50.0
trichloroethylene	1	0.0	44.8	50.0
trichloromethane	3	0.0	42.0	40.9
tridecandioic acid	1	11.0	116.9	131.2
tridecanoic acid	1	11.0	135.5	131.2
tridecanol	1	12.0	148.1	138.6
trifluoroacetonitrile	3	0.0	38.6	40.9
trifluoromethane	3	0.0	34.4	40.9
trifluoromethanethiol	3	0.0	42.5	40.9
trifluoromethyl (2-hydroxy-1-propenyl)ketone	1	0.5	36.4	53.7
trimellitic anhydride(1,2,4-benzenetricarboxylic acid)	1	0.0	27.2	50.0
trimethylamine	1	0.0	41.9	50.0
trimethylhydrazine	1	1.0	47.2	57.4
trinitroglycerine	1	6.5	76.6	98.0
triphenyl phosphate	1	3.0	91.8	72.1
triphenylamine	6	0.0	62.2	35.1
triphenylchloromethane	1	0.0	74.0	50.0
triphenylene	6	0.0	52.5	35.1
triphenylmethane	1	1.5	60.1	61.1
triphenylphosphine oxide	3	0.0	56.1	40.9
tri-tert-butylmethanol	1	0.0	32.6	50.0
undecanedioic acid	1	9.0	103.0	116.4
undecanoic acid	1	8.5	114.2	112.7
undecanolactone	1	7.0	58.0	101.7
urea	2	0.0	31.7	44.3
vinyl acetate	1	1.0	46.8	57.4
vinyl chloride	1	0.0	41.2	50.0
xanthene	2	0.0	51.4	44.3
xanthone	2	0.0	58.1	44.3

Z-3-chloro-2-butenoic acid	1	0.5	56.5	53.7
z-enantholactam	1	6.5	44.4	98.0

APPENDIX D. Experimental and predicted Melting Points (T_m) for 2230 organic compounds.

Name	T_m (K)	
	experimental	predicted
(+)2-butanol	177.4	194.5
(+)a-(3-benzoylphenyl)propionic acid	367.4	409.1
(2,4,5-trichlorophenoxy)acetic acid	431.2	412.6
(2,4-dichlorophenoxy)acetic acid	412.5	396.7
(4-chloro-2-methylphenoxy)acetic acid	392.9	393.1
(4-chloro-o-tolyloxy)acetic acid	392.9	393.1
(d) 1,2-dibromoacenaphthene	416.0	438.6
(d) 1,2-dichloroacenaphthene	375.0	401.6
(d) 1,2-diphenyl-1,2-dihydroxyethane	420.5	398.8
(d) 2-(1-naphthoxy)propionamide	475.0	471.2
(D) 2-(2-chloro-3-methylphenoxy)propionic acid	359.5	398.3
(d) 2-(m-chlorophenoxy)propanoic acid	367.5	386.0
(d) 2-(o-chlorophenoxy)propanoic acid	369.0	386.0
(d) 2-(p-bromophenoxy)propanoic acid	380.0	401.3
(d) 2-(p-methoxyphenyl)propiophenone	326.0	353.1
(d) 2-(p-nitrophenoxy)propanoic acid	362.0	423.2
(d) 2,3-dibromo-1,4-butanediol	388.2	342.6
(d) 2-phenoxypropionic acid	359.0	370.1
(d) 3-(m-bromophenyl)-3-hydroxypropanoic acid	350.0	415.9
(d) 3-(m-chlorophenyl)-3-hydroxypropanoic acid	368.0	400.7
(d) 3-(m-fluorophenyl)-3-hydroxypropanoic acid	311.0	385.1
(d) 3-(o-fluorophenyl)-3-hydroxypropanoic acid	348.0	385.1
(d) 3-(p-bromophenyl)-3-hydroxypropanoic acid	398.0	415.9
(d) 3-(p-chlorophenyl)-3-hydroxypropanoic acid	385.0	400.7
(d) 3-(p-fluorophenyl)-3-hydroxypropanoic acid	381.0	385.1
(d) 3-hydroxy-3-phenylbutyric acid	357.0	394.2
(d) 3-hydroxy-3-phenylvaleric acid	379.0	394.7
(d) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid	431.0	413.4
(d) 3-phenyl-3-hydroxypropanoic acid	391.0	384.8
(d) dimethyl diacetyltartrate	377.2	270.4
(d) dimethyl tartrate	322.2	290.0
(d) malic acid	376.0	425.5
(d) mandelic acid	406.0	380.9
(d) methylenebisthiopropionic acid	355.0	382.7
(d) m-fluoromandelic acid	394.0	381.2
(d) o-chloromandelic acid	392.5	398.8
(d) o-fluoromandelic acid	363.0	381.2
(d) p-chloromandelic acid	394.0	398.8
(d) p-fluoromandelic acid	426.0	381.2
(dl) 1,2-dibromoacenaphthene	397.0	438.6
(dl) 1,2-dichloroacenaphthene	339.0	401.6
(dl) 1,2-diphenyl-1,2-dihydroxyethane	393.0	398.8
(dl) 2-(1-naphthoxy)propionamide	445.0	471.2
(dl) 2-(2-chloro-3-methylphenoxy)propionic acid	391.5	398.3
(dl) 2-(m-chlorophenoxy)propanoic acid	386.0	386.0

(dl) 2-(o-chlorophenoxy)propanoic acid	388.0	386.0
(dl) 2-(p-bromophenoxy)propanoic acid	385.0	401.3
(dl) 2-(p-methoxyphenyl)propiophenone	353.0	353.1
(dl) 2-(p-nitrophenoxy)propanoic acid	411.4	423.2
(dl) 2,3-dibromo-1,4-butanediol	363.2	342.6
(dl) 2-phenoxypropionic acid	388.0	370.1
(dl) 3-(m-bromophenyl)-3-hydroxypropanoic acid	349.0	415.9
(dl) 3-(m-chlorophenyl)-3-hydroxypropanoic acid	340.0	400.7
(dl) 3-(m-fluorophenyl)-3-hydroxypropanoic acid	290.0	385.1
(dl) 3-(o-fluorophenyl)-3-hydroxypropanoic acid	342.0	385.1
(dl) 3-(p-bromophenyl)-3-hydroxypropanoic acid	371.0	415.9
(dl) 3-(p-chlorophenyl)-3-hydroxypropanoic acid	357.0	400.7
(dl) 3-(p-fluorophenyl)-3-hydroxypropanoic acid	362.0	385.1
(dl) 3-hydroxy-3-phenylbutyric acid	330.0	394.2
(dl) 3-hydroxy-3-phenylvaleric acid	394.0	394.7
(DL) 3-methylnonane	188.5	238.7
(dl) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid	407.0	413.4
(dl) 3-phenyl-3-hydroxypropanoic acid	366.0	384.8
(DL) 4-methylnonane	174.7	238.7
(dl) dimethyl diacetyltartrate	355.2	270.4
(dl) dimethyl tartrate	360.2	290.0
(dl) malic acid I	402.0	425.5
(dl) malic acid II	396.0	425.5
(dl) mandelic acid	392.0	380.9
(dl) menthol	301.2	231.6
(dl) methylenebisthiopropionic acid	429.0	382.7
(dl) m-fluoromandelic acid	370.0	381.2
(dl) o-chloromandelic acid	358.5	398.8
(dl) o-fluoromandelic acid	390.0	381.2
(dl) p-chloromandelic acid	394.0	398.8
(dl) p-fluoromandelic acid	403.0	381.2
(l) menthol	316.2	231.6
[(benzoylamino)oxy] acetic acid	416.9	416.9
1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone	351.4	399.4
1-(methylamino)-9,10-anthracenedione	443.2	477.9
1-(o-chlorophenyl)thiourea	413.5	350.4
1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)	382.1	371.1
1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene	360.6	373.3
1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene)	331.6	288.0
1,1'-(2,2-dichloroethylidenebis(4-chlorobenzene)	382.1	341.9
1,1-(di-p-chlorophenyl)-2-nitropropane	354.3	322.0
1,1,1,3-tetrachloropropane	237.7	311.1
1,1,1-trichloro-3,3,3-trifluoropropane	232.7	274.0
1,1,1-trichloroethane	240.1	241.3
1,1,1-trifluoro-3,3-dichloropropane	182.2	205.8
1,1,1-trifluoro-3-chloropropane	179.4	216.0
1,1,1-trifluoroethane	161.9	107.8
1,1,1-trifluoro-n-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide	418.4	427.2
1,1,1-trinitroethane	329.2	266.6
1,1,2,2-tetrachlorodifluoroethane	299.7	251.4
1,1,2,2-tetrachloroethane	230.8	216.6
1,1,2-tribromoethane	244.0	228.4
1,1,2-trichloroethane	237.1	226.8

1,1,2-trifluoro-1,2,2-trichloroethane	236.9	215.1
1,1,3,3-tetraethylurea	253.0	283.4
1,1,3-trimethylurea	344.4	322.6
1,10-decanediol	345.5	342.8
1,12-benzoperylene	554.2	470.7
1,1-bis(4-chlorophenyl)-2-nitrobutane	330.3	329.2
1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene	360.4	381.5
1,1-dichloroethane	176.2	159.5
1,1-dichloroethene	150.9	156.2
1,1-dicyclohexyldodecane	300.6	335.4
1,1-diethylurea	342.3	392.3
1,1-difluoro-1-chloroethane	142.4	124.6
1,1-dimethyl-3-phenylurea	404.8	386.4
1,1-dimethylcyclohexane	239.8	183.6
1,1-dimethylcyclopentane	203.7	168.5
1,1-dimethylurea	454.0	390.3
1,1-diphenyldodecane	281.4	343.9
1,2,3,4,5,6,7,8-octahydroanthracene	345.4	347.8
1,2,3,4,5-pentahydroxypentane (D-Arabitol)	379.4	382.0
1,2,3,4,5-pentahydroxypentane (Ribitol)	374.7	382.0
1,2,3,4,5-pentahydroxypentane (Xylitol)	365.7	382.0
1,2,3,4-tetracarbomethoxybenzene	404.7	389.6
1,2,3,4-tetracarbomethoxynaphthalene	423.7	434.0
1,2,3,4-tetrachlorobenzene	320.0	308.5
1,2,3,4-tetrafluorobenzene	233.3	217.4
1,2,3,4-tetrahydronaphthlene	237.4	279.3
1,2,3,4-tetrahydroquinoline	290.0	297.6
1,2,3,4-tetrahydroxybutane	396.0	353.5
1,2,3,4-tetramethylbenzene	265.4	287.0
1,2,3,5-tetracarbomethoxybenzene	389.2	389.6
1,2,3,5-tetrachlorobenzene	323.9	308.5
1,2,3,5-tetrafluorobenzene	226.9	192.4
1,2,3,5-tetramethylbenzene	248.6	287.0
1,2,3,6,7,8-hexahydropyrene	407.7	483.4
1,2,3-tribromopropane	289.4	300.2
1,2,3-tricarbomethoxybenzene	375.7	339.7
1,2,3-tricarbomethoxynaphthalene	362.7	404.0
1,2,3-trichlorobenzene	326.9	285.2
1,2,3-trihydroxybenzene	407.2	466.9
1,2,3-trihydroxypropane	293.0	325.2
1,2,3-trimethylbenzene	247.8	269.2
1,2,4,5,8,9-tribenzopyrene	608.0	622.3
1,2,4,5-tetrabromobenzene	453.1	457.1
1,2,4,5-tetracarbomethoxybenzene	416.7	389.6
1,2,4,5-tetracarbomethoxynaphthalene	438.2	434.0
1,2,4,5-tetrachloro-3-nitrobenzene	373.3	341.7
1,2,4,5-tetrachlorobenzene	421.2	354.5
1,2,4,5-tetrafluorobenzene	277.0	249.9
1,2,4,5-tetramethylbenzene	352.4	329.9
1,2,4-triazole	393.5	350.5
1,2,4-tricarbomethoxynaphthalene	393.7	404.0
1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene	419.9	450.0
1,2,4-trimethylbenzene	229.3	238.2

1,2,5,6-tetracarbomethoxynaphthalene	470.2	434.0
1,2,5-tricarbomethoxynaphthalene	363.0	404.0
1,2,6,7-tetracarbomethoxynaphthalene	407.2	434.0
1,2,6-tricarbomethoxynaphthalene	416.7	404.0
1,2,7,8-tetrahydroxyoctane	352.2	368.7
1,2,7-tricarbomethoxynaphthalene	427.2	404.0
1,2,8-tricarbomethoxynaphthalene	366.7	404.0
1,2:3,4-dibenzanthracene	553.5	534.5
1,2:3,4-dibenzopyrene	501.2	480.1
1,2:4,5-dibenzopyrene	520.2	480.1
1,2:5,6-dibenzanthracene	544.2	534.5
1,2-benzacenaphthene (fluoranthene)	383.4	338.9
1,2-benzanthracene	434.3	402.5
1,2-benzofluorene	462.8	380.8
1,2-benzopyrene	454.4	462.7
1,2-bromochlorobenzene	260.6	251.6
1,2-bromoiodobenzene	294.2	290.6
1,2-butadiene	136.9	172.1
1,2-chloronitrobenzene	308.2	280.0
1,2-diamino-2-methylpropane	256.1	267.4
1,2-diaminopropane	236.5	270.9
1,2-dibenzoylethane	418.6	388.0
1,2-dibromo-1,1-difluoroethane	206.3	224.9
1,2-dibromobenzene	275.0	306.6
1,2-dibromoethane	283.0	265.6
1,2-dibromotetrafluoroethane	162.8	184.2
1,2-dicarbomethoxybenzene	274.2	295.9
1,2-dicarbomethoxynaphthalene	358.2	367.3
1,2-dichlorobenzene	256.5	262.0
1,2-dichloroethane	237.2	237.0
1,2-dichloropropane	172.7	208.1
1,2-dichloro-tetrafluoroethane	180.6	178.7
1,2-dicyanobenzene	414.1	402.3
1,2-difluoro-2,2-dichloroethane	163.0	225.3
1,2-difluorobenzene	226.0	216.5
1,2-dihydro-6-neopentyl-2-oxonicotinic acid	469.2	469.2
1,2-dihydroxybenzene	376.9	374.5
1,2-diiodobenzene	296.6	350.2
1,2'-dinaphthylmethane	369.6	406.4
1,2-dinitrobenzene	396.1	370.7
1,2-diphenyl-2-(N-piperidinyl)-1-ethanone	349.2	351.5
1,2-diphenylethane	324.3	283.6
1,2-pentadiene	135.9	92.1
1,3,3-trinitroazetidine	375.5	358.4
1,3,5,5-tetranitro-1,3-diazacyclohexane	430.0	429.7
1,3,5,7-tetroxane	385.0	306.0
1,3,5-tri-a-naphthylbenzene	472.0	494.8
1,3,5-tricarbomethoxynaphthalene	402.7	404.0
1,3,5-trichloro-2,4,6-trifluorobenzene	335.0	361.1
1,3,5-trichlorobenzene	336.7	359.2
1,3,5-trimethylbenzene	228.4	339.0
1,3,5-trinitro-1,3,5-triazacyclohexane	478.2	434.0
1,3,5-trinitrobenzene	380.3	396.8

1,3,5-trinitroso-1,3,5-triazacyclohexane	376.0	394.9
1,3,5-trioxane	333.4	276.5
1,3,5-triphenylbenzene	446.0	437.6
1,3,6-trimethyluracil	384.5	374.8
1,3,7-tricarbomethoxynaphthalene	446.7	404.0
1,3,7-trichlorodibenzodioxin	421.7	397.4
1,3,8-tricarbomethoxynaphthalene	388.2	404.0
1,3-bromochlorobenzene	252.0	251.6
1,3-bromoiodobenzene	282.5	290.6
1,3-butadiene	164.2	179.4
1,3-cyclohexadiene	161.0	188.2
1,3-dibromobenzene	266.3	306.6
1,3-dibromopropane	238.6	280.8
1,3-dibutylurea	346.9	368.1
1,3-dicarbomethoxybenzene	341.2	295.9
1,3-dicarbomethoxynaphthalene	378.7	367.3
1,3-dichlorobenzene	248.4	262.0
1,3-dicyanopropane	244.2	298.4
1,3-diethylurea	383.4	355.9
1,3-difluorobenzene	204.0	216.5
1,3-dihydroxybenzene	382.6	383.1
1,3-diiodobenzene	307.4	350.2
1,3-dimethyluracil	398.0	331.5
1,3-dimethylurea	381.0	345.4
1,3-dinitro-1,3-diazacycloheptane	374.0	403.3
1,3-dinitro-1,3-diazacyclohexane	354.0	353.9
1,3-dinitro-1,3-diazacyclopentane	410.0	377.3
1,3-dinitro-5-nitroso-1,3,5-triazacyclohexane	446.0	421.0
1,3-dinitrobenzene	363.2	328.1
1,3-dioxolane	175.9	241.3
1,3-diphenylacetone	307.2	319.6
1,3-diphenylurea	512.0	490.1
1,3-dithiane	327.2	317.4
1,3-nitrochlorobenzene	317.6	280.0
1,4,5,8-tetracarbomethoxynaphthalene	477.2	434.0
1,4,5-tricarbomethoxynaphthalene	402.2	404.0
1,4,6-tricarbomethoxynaphthalene	409.2	404.0
1,4-[bis[(4-methylphenyl)amino]-9,10-anthracenedione	491.2	502.6
1,4-bis(diphenylphosphino)butane	405.9	399.2
1,4-bis(phenylglyoxaloyl)benzene	425.1	408.7
1,4-bis-[4-(4'-n-butylbiphenyl)]butane	464.2	397.8
1,4-bromochlorobenzene	337.8	284.3
1,4-bromoiodobenzene	363.3	328.4
1,4-cyclohexadiene	224.0	244.1
1,4-cyclohexanedione	348.2	276.0
1,4-diamino-2-methoxyanthraquinone	515.2	550.0
1,4-diaminoanthraquinone	484.2	626.1
1,4-dibromobenzene	360.1	352.4
1,4-dicarbomethoxybenzene	413.8	295.9
1,4-dicarbomethoxynaphthalene	340.2	367.3
1,4-dichloro-2,5-dimethoxybenzene	403.9	316.1
1,4-dichlorobenzene	326.0	301.1
1,4-dihydroxybenzene	453.0	440.3

1,4-dihydroxybutane	293.6	307.9
1,4-diiodobenzene	402.0	402.5
1,4-dimethylnaphthalene	279.9	331.0
1,4-dinitrobenzene	446.7	426.1
1,4-dioxane	284.1	248.9
1,4-dioxane-2,5-dione	356.2	379.4
1,4-di-tert-butylbenzene	341.5	321.2
1,4-dithiane	384.6	317.4
1,4-nitrochlorobenzene	354.6	316.3
1,4-pentadiene	124.3	58.5
1,5-cyclooctanedione	341.2	283.3
1,5-dicarbomethoxynaphthalene	392.0	367.3
1,5-dichloro-3-oxapentane	226.5	264.9
1,5-dimethyltetrazole	349.0	273.0
1,5-dinitro-3-nitroso-1,3,5-triazacycloheptane	440.0	411.2
1,5-pentanediol	248.0	316.4
1,6-bis-[4-(4'-ethylbiphenyl)]hexane	422.2	387.2
1,6-dicarbomethoxynaphthalene	371.8	367.3
1,6-hexanediol	314.7	323.5
1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane	422.5	435.2
1,7-dicarbomethoxynaphthalene	363.2	367.3
1,7-heptanediol	295.2	329.4
1,8-bis-(4-biphenyl)octane	415.2	425.9
1,8-bis-[4-(4'-ethylbiphenyl)]butane	454.2	397.3
1,8-bis-[4-(4'-ethylbiphenyl)]octane	413.2	397.8
1,8-bis-[4-(4'-n-butylbiphenyl)]octane	414.2	398.2
1,8-dimethylnaphthalene	336.3	331.0
1,8-octanediol	332.8	334.5
1,9-nonanediol	319.6	338.9
1-[3,5-di-tert-butyl-4-hydroxyphenyl]-5-hexyn-1-one	342.2	425.5
10H-phenothiazine	458.2	497.7
10-nonadecanone	330.0	305.5
10-octadecynoic acid	319.0	307.9
11-cyclohexyleicosane	269.9	340.3
11-heneicosanone	336.7	313.1
11-n-decylheneicosane	282.3	328.9
11-octadecynoic acid	320.0	307.9
11-phenyleicosane	294.3	335.8
12-octadecynoic acid	320.0	307.9
12-tricosanone	342.2	319.5
13-octadecynoic acid	322.0	307.9
14-octadecynoic acid	337.0	307.9
16-octadecynoic acid	347.0	323.1
17-alpha-hydroxyprogesterone caproate	393.2	418.5
17-methyltestosterone	438.0	401.0
17-octadecynoic acid	340.0	344.0
1-8-naphthalic anhydride	542.3	455.5
1a,2a,3ß,4a,5a,6ß-hexachlorocyclohexane	386.8	313.2
1-acetoxynaphthalene	319.2	311.8
1-acetyl-2-naphthol	337.0	393.0
1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione	458.2	592.7
1-aminoanthraquinone	524.2	509.7
1-aminopropane	188.4	205.7

1-benzoyl-2-naphthol	414.1	409.9
1-bromo-2-chloro-1,1,2-trifluoroethane	146.2	168.7
1-bromo-2-chloroethane	256.4	251.3
1-bromobutane	160.4	235.9
1-bromodocosane	317.2	333.4
1-bromoheptane	214.4	277.6
1-bromohexane	188.1	266.3
1-bromonaphthalene	271.4	301.6
1-bromononane	243.2	295.3
1-bromooctane	218.2	287.1
1-bromopentane	185.1	252.6
1-bromotricosane	339.6	348.2
1-bromoundecane	263.3	308.5
1-butene	87.8	83.6
1-butyne	147.4	134.2
1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene	345.8	371.1
1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene	349.8	337.6
1-chloro-2,2-(bis-(4-chlorophenyl)ethylene	337.9	347.0
1-chlorodibenzodioxin	378.2	356.3
1-chloronaphthalene	270.7	281.9
1-cis-3-pentadiene	132.4	171.5
1-cyclohexyl-1-phenyldodecane	275.8	355.5
1-decanethiol	247.9	276.5
1-decanol	280.1	307.3
1-decene	206.9	226.4
1-deoxy-D-glucopyranose	403.2	415.0
1-docosanol	345.2	336.1
1-dodecene	237.9	241.2
1H-1,2,4-triazol-3-amine	428.3	420.7
1-heptanethiol	229.9	245.1
1-heptanol	240.4	283.8
1-heptene	154.3	175.9
1-hexacosanol	351.7	344.0
1-hexadecanol	322.2	318.6
1-hexadecene	277.5	273.2
1-hexanethiol	192.6	230.8
1-hexanol	225.8	273.1
1-hexene	133.4	151.7
1-iodonaphthalene	280.0	320.9
1-methoxy-2-(2,2,2-tricloro-1-(4-methoxyphenyl)ethyl)benzene	347.6	373.3
1-methyl-7-isopropylphenanthrene	369.0	333.4
1-methyl-9H-pyrido[3,4-b]indole	509.9	465.8
1-methylcyclohexanol	299.2	218.0
1-methylcyclopentanol	310.2	206.9
1-methylnaphthalene	242.7	277.1
1-methyltetrazole	315.0	257.2
1-naphthaleneacetamide	455.5	446.7
1-naphthaleneacetic acid	405.3	394.1
1-naphthoic acid	435.2	455.3
1-naphthyl benzoate	329.2	413.9
1-naphthyl methylcarbamate	416.3	383.8
1-naphthylamine	323.2	331.6
1-nitronaphthalene	329.9	330.0

1-nonanethiol	267.7	267.5
1-nonene	191.6	212.3
1-octanethiol	224.0	257.2
1-octene	171.5	195.7
1-pentadecanol	316.6	314.7
1-pentanethiol	197.5	213.5
1-pentanol	195.6	260.1
1-pentene	107.9	121.8
1-propanethiol	160.0	165.7
1-propanol	148.8	224.3
1-tetradecanol	311.0	310.4
1-undecene	224.0	238.5
2-((4-chloro-6-(cyclopropylamino)-1,3,5-triazin-2-yl)amino-2-methylpropanenitrile	438.5	542.3
2-(1,3-dioxolan-2-yl)phenyl methylcarbamate	387.2	468.8
2-(1'-cyclohexenyl)cyclohexanone	278.8	226.9
2-(1-methylethyl)phenyl methylcarbamate	369.3	319.8
2-(2,4,5-trichlorophenoxy)propanoic acid	450.6	417.8
2-(2,4-dichlorophenoxy)propanoic acid	389.2	401.9
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	396.3	396.3
2-(3-hydroxy-2-quinolinyl)-1H-indene-1,3(2H)-dione	539.2	564.6
2-(4-chloro-2-methylphenoxy)propanoic acid	366.2	398.3
2-(6-methoxy-2-naphthyl)propionic acid	439.2	399.0
2-(dimethylamino)-1,2-diphenylethanone	334.2	340.1
2-(docosanoxy)ethanol	335.9	336.2
2-(hexadecyloxy)ethanol	318.5	320.8
2,11-dicyclohexyldodecane	300.6	337.8
2,2,2-trinitroethanol	344.9	343.8
2,2,2-trinitroethyl 4,4,4-trinitrobutyrate	366.5	476.0
2,2,2-trinitroethyl-4,4-dinitropentanoate	366.7	367.2
2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	455.8	542.1
2,2',3,3',5,5',6,6'-octachlorobiphenyl	433.8	596.3
2,2',3,3',5,5',6-heptachlorobiphenyl	395.4	438.6
2,2',3,3',5,5'-hexachlorobiphenyl	424.9	472.3
2,2',3,3',6,6'-hexachlorobiphenyl	385.2	418.0
2,2,3,3-tetramethylbutane	373.9	368.5
2,2,3,3-tetramethylpentane	263.4	277.0
2,2,3-trimethylbutane	247.7	190.5
2,2',4,4',6,6'-hexachlorobiphenyl	386.7	542.8
2,2,4,4-tetramethylpentan-3-ol	322.0	352.7
2,2,4,4-tetramethylpentane	206.7	317.9
2,2',4,5,5'-pentachlorobiphenyl	350.1	397.4
2,2',4',5-tetrachlorobiphenyl	339.1	376.8
2,2,4-trimethylpentane	165.8	217.4
2,2,5,5-tetramethylhex-3-ene	268.9	201.8
2,2,6,6-tetramethyl-1,3-dioxane	250.6	228.5
2,2-bis-(4-cyanatophenyl)propane	355.8	355.8
2,2-bis(phenylthio)propane	329.0	375.2
2,2-bis-hydroxymethylpropanoic acid	468.0	415.1
2,2-dichloropropane	239.3	227.9
2,2-dicyanopropane	307.5	253.7
2,2-dimethoxy-1,2-diphenylethanone	338.5	293.7
2,2-dimethyl-1,3-dioxan	229.6	238.7
2,2-dimethyl-1,3-propanediol	403.2	366.5

2,2-dimethyl-1-propanol	264.0	292.7
2,2-dimethylbutane	174.3	223.7
2,2-dimethylheptane	160.0	277.6
2,2-dimethylpentane	148.1	246.3
2,2-dimethylpropane	256.5	280.2
2,2-dimethylpropanoic acid (pivalic acid)	309.1	312.4
2,2-dinitro-1,3-propanediol	341.2	355.5
2,2-dinitropropane	324.5	204.5
2,2-dinitropropanol	366.7	289.7
2,2-dinitropropyl-4,4-dinitropentanoate	370.8	335.5
2,2-dintropropyl-4,4,4-trinitrobutyrate	368.2	353.9
2,2'-methylenebis(3,4,6-trichlorophenol)	437.6	513.6
2,3,4,5,6-pentachlorobiphenyl	397.6	449.1
2,3,4,5,6-pentafluorotoluene	243.7	235.8
2,3,4,5-tetrachlorobiphenyl	363.9	376.8
2,3,4-trimethylpentane	163.6	114.2
2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione	567.2	605.8
2,3,5-tricarbomethoxynaphthalene	401.7	404.0
2,3,5-triiodobenzoic acid	503.8	537.7
2,3,6,7,10,11-hexakis(1-decynyl)triphenylene	314.2	358.4
2,3,6,7-tetracarbomethoxynaphthalene	458.2	434.0
2,3,6-tricarbomethoxynaphthalene	399.2	404.0
2,3,6-trichlorobenzoic acid	402.7	394.6
2,3,6-trichlorophenylacetic acid	432.3	386.4
2,3-benzofluorene	489.7	380.8
2,3-dicarbomethoxynaphthalene	324.2	367.3
2,3-dichloro-1,4-naphthalenedione	469.0	492.6
2,3-dichlorophenol	330.0	302.2
2,3-dihydro-2,2-dimethyl-7-benzofuranol-3-one	440.6	412.1
2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	426.2	412.9
2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide	401.5	401.5
2,3-dimethyl-2,3-bis(4-tert-butylphenyl)butane	493.0	441.6
2,3-dimethyl-2,3-bis(phenylazo)butane	342.3	391.1
2,3-dimethyl-2,3-butanediol	316.2	312.3
2,3-dimethyl-2,3-diphenylbutane	392.0	340.8
2,3-dimethyl-2-butene	198.9	253.6
2,3-dimethylbenzoic acid	417.6	416.4
2,3-dimethylbutane	145.2	106.4
2,3-dimethylnaphthalene	378.0	331.0
2,3-dimethylphenol	346.0	296.5
2,3-dimethylpyridine	258.6	238.4
2,3-dinitrophenol	417.0	376.4
2,3-dinitrotoluene	329.8	343.9
2,3-pentadiene	147.5	222.6
2,4,4-trimethyl-1-pentene	178.9	214.4
2,4,4-trimethyl-2-pentene	166.0	198.5
2,4,5,6-tetrachloro-1,3-benzenedicarbonitile	526.2	495.3
2,4,5-tribromostyrene	340.3	342.0
2,4,5-trichlorobiphenyl	349.5	356.3
2,4,5-trichlorophenol	340.3	322.8
2,4,5-trimethylthiazole	240.7	254.5
2,4,5-trinitrotoluene	376.2	412.6
2,4,6,N-tetranitro-N-methyltoluidene	375.6	458.4

2,4,6-N-tetranitroethylaniline	369.0	494.6
2,4,6-tribromophenol	366.2	378.2
2,4,6-trichlorobiphenyl	334.3	402.6
2,4,6-trimethyl-1,3,5-trioxane	285.7	359.7
2,4,6-trimethylpyridine	229.0	254.3
2,4,6-trinitro-1,3-dimethylbenzene	455.4	428.5
2,4,6-trinitroresorcinol	454.8	441.5
2,4,6-trinitrotoluene	352.2	466.2
2,4,6-tri-tert-butylphenol	405.2	460.7
2,4,7-trinitrofluoren-9-one	449.2	397.1
2,4-dibromophenol	313.0	341.7
2,4-dichlorophenol	318.0	302.2
2,4-dichlorophenyl 4-nitrophenyl ether	342.0	371.6
2,4-dimethylpentane	154.0	139.8
2,4-dimethylpyridine	209.4	238.4
2,4-dimethylpyrrole	268.5	324.3
2,4-dimethylthiazole	222.9	269.7
2,4-dinitrochlorobenzene	325.2	348.7
2,4-dinitrophenol	388.0	376.4
2,4-dinitrotoluene	343.3	343.9
2,4-di-tert-butylthiazole	258.2	337.6
2,4-hexadiyne	341.7	182.4
2,5,8,11-tetraoxadodecane	229.3	236.1
2,5,8-trioxanonane	209.1	212.4
2,5-dibutoxy-1,4-benzoquinone	473.3	395.0
2,5-dichlorophenol	331.0	302.2
2,5-diethoxy-1,4-benzoquinone	459.3	393.2
2,5-dimethylaniline	279.0	292.6
2,5-dimethylphenol	348.0	296.5
2,5-dimethylpyridine	259.1	238.4
2,5-dimethylpyrrole	280.9	366.5
2,5-dimethyltetrazole	256.4	273.0
2,5-dimethylthiophene	210.6	251.6
2,5-di-n-heptadecyloxy-1,4-benzoquinone	395.3	395.5
2,5-di-n-heptyloxy-1,4-benzoquinone	406.2	391.6
2,5-di-n-hexadecyloxy-1,4-benzoquinone	394.2	395.3
2,5-di-n-hexyloxy-1,4-benzoquinone	412.1	395.9
2,5-dinitrophenol	381.0	376.4
2,5-di-n-nonadecyloxy-1,4-benzoquinone	396.2	395.8
2,5-di-n-nonyloxy-1,4-benzoquinone	402.7	392.9
2,5-di-n-octyloxy-1,4-benzoquinone	405.8	392.3
2,5-di-n-pentadecyloxy-1,4-benzoquinone	393.5	395.0
2,5-di-n-undecyloxy-1,4-benzoquinone	397.2	393.8
2,5-dipentoxy-1,4-benzoquinone	414.6	395.5
2,5-dipropoxy-1,4-benzoquinone	460.8	394.2
2,6-dichloro-4-benzenamine	467.2	341.4
2,6-dichloro-4-nitroaniline	466.8	410.4
2,6-dichlorobenzonitrile	417.2	355.4
2,6-dichlorobiphenyl	307.9	379.3
2,6-dichlorophenol	340.0	337.2
2,6-diisopropylphenol	292.8	274.0
2,6-dimethylnaphthalene	383.3	331.0
2,6-dimethylphenol	318.9	335.1

2,6-dimethylpyridine	267.1	269.4
2,6-dinitrochlorobenzene	361.2	348.7
2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	321.4	278.6
2,6-dinitrophenol	336.0	350.5
2,6-dinitrotoluene	327.5	343.9
2,6-di-tert-butyl-4-methoxyphenol	374.4	440.1
2,6-di-tert-butyl-4-methylphenol	343.7	411.3
2,6-di-tert-butylphenol	310.7	395.4
2,7-dicarbomethoxynaphthalene	410.2	367.3
2,7-dimethylnaphthalene	368.8	331.0
2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	454.2	455.9
2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	476.0	438.7
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	437.9	491.3
2-[bis(2-chloroethyl)amino]tetrahydro-2H-1,3,2-oxazophosphorine-2-oxide	322.6	322.6
2-acetoxynaphthalene	342.2	311.8
2-acetyl-1-naphthol	371.8	418.9
2-acetylamino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	490.2	541.2
2-acetylamino-9-[(2-hydroxyethoxy)methyl]-9H-purine	454.2	476.3
2-amino-2-hydroxymethylpropane-1,3-diol	407.5	404.8
2-amino-2-methylpropane-1,3-diol	384.0	352.2
2-amino-9-[(2-acetoxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	515.2	511.6
2-amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	528.2	509.3
2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine	462.2	434.8
2-aminobenzoic acid	417.8	403.2
2-aminobiphenyl	322.3	364.8
2-aminopropane	178.0	143.9
2-benzoyl-1-naphthol	343.9	435.8
2-bromo-2-chloro-1,1,1-trifluoroethane	154.7	193.6
2-bromobutane	160.3	186.0
2-bromonaphthalene	329.0	301.6
2-bromopropane	184.1	154.5
2-bromothiophene	203.9	231.3
2-butanethiol	133.0	136.8
2-butanol	184.7	194.5
2-butanone	186.5	176.0
2-butyne	240.9	131.1
2-carbomethoxynaphthalene	350.2	321.1
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	358.8	305.4
2-chloro-2-nitropropane	261.6	253.3
2-chloro-6-(trichloromethyl)pyridine	337.8	325.2
2-chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene	370.3	320.3
2-chloroanthraquinone	483.0	485.9
2-chlorobenzoic acid	413.4	379.4
2-chlorobiphenyl	304.9	315.1
2-chlorodibenzodioxin	362.2	356.3
2-chloroethylphosphonic acid	347.9	347.9
2-chloro-n-(2,6-diethylphenyl)-n-(methoxymethyl)acetamide	315.9	271.9
2-chloronaphthalene	332.0	281.9
2-chloro-N-isopropyl N-phenylacetamide	351.4	271.5
2-chloro-N-isopropylacetamide	351.3	294.2
2-chlorophenol	283.0	281.6
2-chloropropane	156.0	138.1
2-chlorothiophene	201.3	211.5

2-cyano-2-methylpropane	292.1	236.1
2-cyclohexyl-4,6-dinitrophenol	378.7	408.1
2-cyclohexylcyclohexanone	277.0	222.4
2-deoxy-2-fluoro-D-glucopyranose	427.2	409.7
2-deoxy-D-glucopyranose	398.7	415.0
2-ethoxyisonitrosoacetanilide	405.0	447.5
2-ethyl-2-diphenylmethyl-1,3-cyclopentanedione	382.2	489.1
2-fluorenyl-2-methyl-1,3-cyclohexanedione	448.2	434.1
2-fluorenyl-2-methyl-1,3-cyclopentanedione	395.2	420.5
2-fluorotoluene	210.7	207.0
2-heneicosanone	333.9	325.8
2-heptanone	237.7	241.3
2-hexadecanoyloxy-1,3-bis-(9-cis-octadecenoyloxy)propane	291.9	341.4
2-hexanone	217.7	224.2
2-hydroxybenzoic acid	431.8	407.1
2-hydroxymethyl-2-methyl-1,3-propanediol	470.0	423.5
2-iodobenzoic acid	435.1	418.4
2-iodonaphthalene	327.6	320.9
2-isopropoxyphenyl N-methylcarbamate	363.1	332.9
2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide	327.9	322.2
2-methyl-1,3-butadiene	127.3	138.2
2-methyl-1-butene	135.6	126.7
2-methyl-1-phenyl-2-(N-piperidinyl)-1-propanone	310.2	332.1
2-methyl-1-propanol	171.2	195.4
2-methyl-2-(methylsulfonyl)propanal oxime	382.0	373.9
2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime	374.0	353.7
2-methyl-2-butanethiol	146.1	166.7
2-methyl-2-butanol	264.0	211.1
2-methyl-2-butene	139.4	149.1
2-methyl-2-diphenylmethyl-1,3-cyclopentanedione	394.2	393.3
2-methyl-2-nitro-1,3-propandiol	424.0	360.9
2-methyl-2-nitro-1-propanol	361.0	295.8
2-methyl-2-nitropropyl-4,4,4-trinitrobutyrate	349.4	357.8
2-methyl-4,6-dinitrophenol	359.3	392.2
2-methylbutane	113.4	120.5
2-methylcyclothiapentane	172.4	238.7
2-methyldecane	224.3	250.4
2-methylfuran	181.9	193.9
2-methylheptane	164.2	208.9
2-methylhexane	154.9	189.4
2-methylnaphthalene	307.7	277.1
2-methylnonane	198.8	238.7
2-methylpentane	119.6	165.4
2-methylpiperidine	269.4	199.2
2-methylpyridine	206.5	222.6
2-methyltetrazole	286.0	257.2
2-methylthiazole	248.6	222.9
2-methylthiophene	207.8	206.8
2-naphthoic acid	460.2	455.3
2-naphthyl benzoate	381.2	413.9
2-naphthylamine	386.2	331.6
2-n-butyl-5-(4-bromobiphenyl-4-yl)thiophene	501.4	385.8
2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	364.6	278.4

2-nitro-5-methylphenol	302.8	323.5
2-nitroaniline	344.4	303.8
2-nonadecanone	328.0	319.3
2-n-propyl-5-(4-bromophenyl)thiophene	360.4	406.2
2-octanone	252.9	255.3
2-pentadecanone	312.2	302.3
2-pentanol	200.0	217.8
2-pentanone	196.3	203.0
2-phenylbenzimidazole	572.2	545.9
2-piperadone	342.3	341.3
2-propanethiol	142.6	98.0
2-propanol	185.2	164.2
2-pyrrolidone	299.0	344.5
2-sec-butyl-4,6-dinitrophenol	313.7	363.8
2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate	341.3	371.1
2-tetradecanone	306.7	296.8
2-undecanone	290.5	285.6
3-(1-methylethyl)-(1H)-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide	412.5	412.5
3-(3,4-dichlorophenyl)-1,1-dimethylurea	429.7	418.2
3-(4-chlorophenyl)-1,1-dimethylurea	447.6	402.3
3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	408.9	396.6
3(n-decylamino)-1,2-propanediol	346.6	334.4
3(n-decyloxy)-1,2-propanediol	311.0	312.9
3(n-decylthio)-1,2-propanediol	311.9	321.4
3(n-dodecylamino)-1,2-propanediol	351.9	340.4
3(n-dodecyloxy)-1,2-propanediol	323.0	320.8
3(n-dodecylthio)-1,2-propanediol	325.5	328.5
3(n-heptylamino)-1,2-propanediol	324.9	343.2
3(n-heptyloxy)-1,2-propanediol	246.2	316.2
3(n-heptylthio)-1,2-propanediol	292.5	326.9
3(n-hexyloxy)-1,2-propanediol	272.9	310.6
3(n-hexylthio)-1,2-propanediol	290.8	322.0
3(n-nonylamino)-1,2-propanediol	343.2	349.5
3-(n-nonyloxy)-1,2-propanediol	297.2	325.6
3(n-octylamino)-1,2-propanediol	335.9	346.6
3(n-octyloxy)-1,2-propanediol	296.1	321.2
3(n-octylthio)-1,2-propanediol	306.5	331.2
3(n-tetradecylamino)-1,2-propanediol	356.2	345.3
3(n-tetradecyloxy)-1,2-propanediol	331.3	327.4
3(n-tetradecylthio)-1,2-propanediol	336.4	334.5
3(n-tridecylamino)-1,2-propanediol	354.9	343.0
3(n-tridecyloxy)-1,2-propanediol	324.2	324.3
3(n-tridecylthio)-1,2-propanediol	330.6	331.7
3(n-undecylamino)-1,2-propanediol	348.8	337.5
3(n-undecyloxy)-1,2-propanediol	311.7	317.0
3(n-undecylthio)-1,2-propanediol	317.4	325.1
3-(p-tolyl-4-sulfonyl)-1-butyl urea	404.8	382.0
3,3',4'4'-tetraaminodiphenyl ether	425.1	507.6
3,3',5,5'-tetra-tert-butyldiphenylmethane-4,4'-diol	447.7	422.7
3,3'-bis-(1-cyclohexylethyl)-5,5'-dimethyldiphenylmethane-2,2'-diol	400.7	432.8
3,3-bis-(chloromethyl)oxacyclobutane	292.2	318.9
3,3-diethylpentane	240.1	251.9

3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime	330.2	321.2
3,3-dimethyl-1-butene	158.4	126.9
3,3-dimethyl-2-butanone	221.7	226.1
3,3-dimethylpentane	138.2	218.2
3,3-dimethylpentanedioic anhydride	396.2	365.5
3,3'-di-tert-butyl-5,5'-dimethyl-2,2-dihydroxydiphenylmethane	403.7	440.6
3,4-benzophenanthrene	334.7	402.5
3,4-benzopyrene	454.2	409.5
3,4-dichloro-2-methoxybenzoic acid	412.5	412.4
3,4-dichlorophenol	341.0	306.0
3',4'-dichloropropionanilide	363.7	372.7
3,4-diethyl-3,4-bis(4-tert-butylphenyl)hexane	400.0	370.4
3,4-dimethylisoxazol 5-sulphanylamide	448.2	467.9
3,4-dimethylphenol	334.0	296.5
3,4-dimethylphenyl methylcarbamate	350.8	353.7
3,4-dimethylpyridine	262.7	238.4
3,4-dinitrophenol	407.0	402.3
3,4-dinitrotoluene	329.5	343.9
3,5,6-trichloro-2-pyridinol	448.1	338.8
3,5,6-trichloro-2-pyridinyloxyacetic acid	423.3	425.0
3,5-dibromo-4-hydroxybenzonitrile	464.0	475.2
3,5-dichlorobenzoic acid	459.3	481.2
3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	428.4	409.7
3,5-dichlorophenol	341.0	345.8
3,5-diisopropylphenol	326.3	274.0
3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate	361.7	355.6
3,5-dimethylbenzoic acid	442.9	470.5
3,5-dimethylphenol	336.8	335.1
3,5-dimethylpyridine	266.9	269.4
3,5-dinitrobenzoic acid	480.4	522.1
3,6-dichloro-2-methoxybenzoic acid	386.7	412.4
3,6-dichloro-5-hydroxy-2-methoxybenzoic acid	409.8	454.4
3-amino-2,5-dichlorobenzoic acid	475.6	466.4
3-aminoacetophenone	371.2	344.4
3-aminobenzoic acid	452.9	455.0
3-bromopentane	167.3	210.3
3-chloro-1,1,1,3,3-pentafluoropropane	165.4	201.3
3-chlorobenzoic acid	427.4	405.3
3-chlorophenol	305.8	285.4
3-deoxy-3-fluoro-D-glucopyranose	378.2	409.7
3-deoxy-D-glucopyranose	387.2	415.0
3-diphenylmethyl-2,4-pentanedione	387.2	382.3
3-ethyl-3-diphenylmethyl-2,4-pentanedione	388.2	370.7
3-ethylheptane	158.0	225.0
3-ethylpentane	154.6	189.4
3-fluorotoluene	184.0	207.0
3-heptanone	236.0	210.5
3-hexanone	217.7	190.1
3-hydroxybenzoic acid	475.1	458.9
3-iodobenzoic acid	460.4	444.3
3-methyl-1,2-butadiene	159.5	150.0
3-methyl-1-butanethiol	139.6	166.7
3-methyl-1-butene	104.7	89.9

3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate	324.3	376.7
3-methyl-2-butanethiol	146.1	107.9
3-methyl-3-diphenylmethyl-2,4-pentanedione	352.2	367.4
3-methylcyclothiapentane	192.0	238.7
3-methylheptane	152.6	208.9
3-methylpentane	110.3	165.4
3-methylpyridine	255.0	222.6
3-methylthiophene	204.2	206.8
3-nitroaniline	387.2	329.7
3-nitrophthalic anhydride	436.2	401.2
3-nitrotoluene	288.7	275.2
3-pentanol	204.2	217.8
3-pentanone	234.2	164.8
3-propyl-3-diphenylmethyl-2,4-pentanedione	349.2	373.4
4-(1,1-dimethylethyl)-n-(1-methylpropyl)-2,6-dinitrobenzeneamine	338.8	283.9
4-(2,4,5-trichlorophenoxy)butanoic acid	386.7	410.2
4-(2,4-dichlorophenoxy)butyric acid	391.4	397.2
4-(2-chlorophenylhydrazone)-3-methyl-5-isoxazolone	440.4	440.4
4-(4-chloro-2-methylphenoxy)butanoic acid	373.4	394.3
4-(4-nitrophenylazo)aniline	488.2	396.4
4-(6-hexenyloxy)-3',4'difluorodiphenyldiacetylene	370.0	350.6
4-(cis-3-hexenyloxy)-3',4'difluorodiphenyldiacetylene	364.6	332.7
4-(cis-4-hexenyloxy)-3',4'difluorodiphenyldiacetylene	364.4	362.0
4-(dipropylamino)-N,N-dimethyl-3,5-dinitrobenzenesulfonamide	413.6	403.7
4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide	414.8	398.3
4,4'-di-(2-methoxyethoxy)biphenyl	412.4	342.7
4,4'dichlorodiphenylsulphone	422.0	408.8
4,4'-didecanoyloxydiphenyldiacetylene	403.0	376.9
4,4'-didodecanoyloxydiphenyldiacetylene	401.0	380.0
4,4'dihydroxydiphenyl-2,2-propane	433.0	384.9
4,4'-dinitrodiphenyl ether	418.2	395.6
4,4'-diundecanoyloxydiphenyldiacetylene	399.0	378.6
4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	431.0	400.1
4[p-[bis(2-chloroethyl)amino]benzene]butanoic acid	338.9	393.0
4'4'-diaminodiphenyl ether	465.4	398.4
4-acetoxybenzoic acid	467.2	394.0
4-amino-6-(1,1-dimethylethyl)-3-(methylthio)1,2,4-triazin-5(4H)-one	399.4	399.4
4-aminoacetophenone	379.2	344.4
4-aminobenzoic acid	461.4	514.1
4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide	453.4	466.9
4-aminopyridine	429.9	313.0
4-benzoyl-1-naphthol	440.6	435.8
4-bromo-2,5-dichloroaniline	343.4	338.6
4-bromo-2,5-dichlorophenol	343.4	342.5
4-bromophenol	336.0	344.8
4-chloroazobenzene	361.2	380.2
4-chlorobenzoic acid	512.9	457.9
4-chlorobiphenyl	348.6	356.0
4-chlorobut-2-ynyl 3-chlorophenylcarbamate	344.1	320.1
4-chlorophenol	315.9	322.5
4-chlorophenoxyacetic acid	429.6	380.8
4-chlorophenyl 4-chlorobenzenesulfonate	360.0	355.1
4-chlorophenylbenzenesulfonate	332.2	337.1

4-ethoxy-4'fluorodiphenyldiacetylene	400.2	364.1
4-ethoxy-4'-trifluoromethyldiphenyldiacetylene	424.9	394.4
4-ethoxybenzoic acid	472.8	402.1
4-ethoxyisonitrosoacetanilide	490.0	447.5
4-ethoxyphenylacetic acid	360.2	358.8
4-ethylbenzoic acid	386.2	359.8
4-ethynyl-1-[(4-ethynylphenyl)methoxy]benzene	371.2	402.8
4-fluorotoluene	216.5	233.9
4-heptanone	240.2	210.5
4-hexylresorcinol	341.5	362.4
4-hydroxy-3,5-diiodobenzonitrile	482.9	518.8
4-hydroxyazobenzene	425.2	440.8
4-hydroxybenzoic acid	488.1	518.5
4-hydroxyphenylacetic acid	423.6	397.2
4-hydroxyphenylpropionic acid	402.5	384.4
4-iodobenzoic acid	543.8	502.1
4-methoxybenzoic acid	457.8	402.4
4-methoxyphenol	328.4	318.5
4-methoxyphenylacetic acid	358.1	281.3
4-methoxyphenylbutyric acid	330.9	352.0
4-methoxyphenylpropionic acid	376.9	347.1
4-methyl-7-aminocoumarin	499.9	442.9
4-methyl-7-diethylaminocoumarin	343.8	354.0
4-methyl-7-dimethylaminocoumarin	416.1	453.3
4-methyl-7-hydroxycoumarin	460.7	446.8
4-methylcyclohex-1-ene	153.6	181.2
4-methylheptane	152.2	208.9
4-methylpent-1-ene	118.9	94.7
4-methylphenanthrene	324.9	347.7
4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline	424.3	413.6
4-methylthiazole	229.1	222.9
4-methylthio-3,5-xylyl methylcarbamate	393.8	364.7
4-n-butoxy-2',3',4'-trifluorodiphenylacetylene	344.4	355.0
4-n-butoxy-4'-fluorodiphenylacetylene	346.7	354.4
4-n-butoxy-4'-trifluoromethyldiphenyldiacetylene	414.3	332.4
4-n-butoxybenzoic acid	432.2	401.6
4-n-butyl-3',4'-difluorodiphenylacetylene	323.5	316.2
4-n-butyl-3',4'-difluorodiphenyldiacetylene	340.8	334.1
4-n-butyl-4'-fluorodiphenylacetylene	329.9	315.9
4-n-ethoxy-2',3',4'-trifluorodiphenylacetylene	356.8	344.8
4-n-ethoxy-2',4'-difluorodiphenylacetylene	343.4	344.5
4-n-ethoxy-4'-fluorodiphenylacetylene	354.4	344.1
4-n-ethyl-3',4'-difluorodiphenylacetylene	301.2	294.7
4-n-hexyl-3',4'-difluorodiphenylacetylene	314.9	345.2
4-n-hexylbenzoic acid	380.0	373.3
4-n-hexyloxy-2',3',4'-trifluorodiphenylacetylene	322.0	361.9
4-n-hexyloxy-2',4'-difluorodiphenylacetylene	320.9	361.7
4-n-hexyloxy-3',4'-difluorodiphenylacetylene	323.6	361.7
4-n-hexyloxy-4'-trifluoromethyldiphenyldiacetylene	394.8	342.2
4-nitro-4'-methylbenzylidene aniline	402.0	283.5
4-nitro-5-methylphenol	401.0	349.4
4-nitroaniline	420.2	372.5
4-nitrophthalic anhydride	388.2	401.2

4-nitrotoluene	324.8	311.0
4-n-octyloxy-N-(3,5-dimethoxybenzylidene)aniline	316.3	357.4
4-n-octyloxy-N-(3,5-dimethylbenzylidene)aniline	324.7	349.6
4-n-octyloxy-N-(4-methoxybenzylidene)aniline	377.3	346.9
4-n-pentoxy-2',3',4'-trifluorodiphenylacetylene	315.8	358.7
4-n-pentoxy-4'-fluorodiphenylacetylene	330.9	358.2
4-n-pentoxybenzoic acid	422.2	401.4
4-n-pentyl-3',4'-difluorodiphenylacetylene	323.1	323.9
4-n-pentyl-3',4'-difluorodiphenyldiacetylene	355.1	340.2
4-n-pentyl-4'-fluorodiphenylacetylene	337.4	323.6
4-n-pentylbenzoic acid	395.0	370.8
4-n-propoxy-2',3',4'-trifluorodiphenylacetylene	327.3	350.4
4-n-propoxy-2',4'-difluorodiphenylacetylene	326.9	350.1
4-n-propoxy-4'-fluorodiphenylacetylene	356.8	349.8
4-n-propoxybenzoic acid	426.7	401.8
4-n-propyl-3',4'-difluorodiphenylacetylene	311.0	306.7
4-n-propyl-3',4'difluorodiphenyldiacetylene	343.7	326.6
4-n-propyl-4'-fluorodiphenylacetylene	324.0	306.3
4-octadecynoic acid	348.0	307.9
4-oxaheptane	158.4	212.3
4-propoxy-4'-trifluoromethyldiphenyldiacetylene	315.9	326.2
4-propylbenzoic acid	422.0	364.3
4'-propylbiphenyl-4-carbonitrile	338.8	358.5
4-tert-butylbenzoic acid	440.0	450.0
4-tert-butylphenol	373.2	330.1
4-trans-(3-fluoro-4-cyanophenyl)cyclohexyl (E)-but-2-enoate	393.2	364.5
4-trans-(4-bromophenyl)cyclohexyl (E)-2-butenoate	388.2	339.9
4-trans-(4-chlorophenyl)cyclohexyl (E)-2-butenoate	386.2	328.6
4-trans-(4-fluorophenyl)cyclohexyl (E)-2-butenoate	354.2	317.0
4-trans-(4-fluorophenylethyl)cyclohexyl (E)-butenoate	335.2	320.6
4-trans-(trifluoromethoxyphenyl)cyclohexyl (E)-but-2-enoate	340.2	342.2
4-trans-cyanocyclohexyl (E) 2-butenoate	366.2	318.8
5'-(trifluoromethanesulphonamide)acet-2',4-xylidide	457.3	487.0
5,5-bis(3,3-dimethylbutyl)2,2,8,8-tetramethylnonane	472.7	347.2
5,5-dimethylperhydro-1,3-oxazine-2-one	440.1	440.1
5,6,7,8-tetrahydroquinoline	222.7	293.3
5,6-dibutyl-5,6-bis(4-tert-butylphenyl)decane	386.0	380.6
5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid	436.6	399.1
5-amino-4-chloro-2-phenyl-3(2H)-pyridazinone	479.2	479.2
5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione	428.3	411.1
5-butyl-2-ethylamino-6-methylpyrimidin-4-ol	432.5	399.9
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione	448.0	469.0
5-isopropyl-m-tolyl methylcarbamate	361.3	330.8
5-methyl N-(methylcarbamoyloxy)thioacetimidate	352.7	351.9
5-methyl-1,2,4-triazolo[3,4-b]benzothiazole	460.2	343.5
5-methylnonane	186.7	238.7
5-methyltetrazole	418.0	434.0
5-methylthiazole	232.8	222.9
5-nonanone	223.2	241.3
5-octadecynoic acid	325.0	307.9
6-(4-biphenyl)-1-hexene	274.5	289.2
6,8,9-trimethyladenine	438.0	450.1
6,9-dimethyl-8-butyladenine	409.2	404.6

6-deoxy-6-fluoro-D-glucopyranose	412.2	408.9
6-deoxy-D-glucopyranose	409.2	364.3
6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one	443.2	443.2
6-octadecynoic acid	324.0	307.9
7,8-benzoquinoline	324.1	347.9
7-octadecynoic acid	322.0	307.9
8-(4-biphenyl)-1-octene	291.5	306.5
8-[4-(4'-n-butylbiphenyl)]-1-octene	315.6	310.9
8-octadecynoic acid	320.0	307.9
9-fluorenone	356.4	414.5
9-heptadecanone	323.9	296.4
9H-pyrido[3,4-b]indole	471.5	449.9
9-methylfluorene	319.2	225.8
9-octadecynoic acid	319.0	307.9
a-(trifluoromethoxy)-a,a-difluoromethyl acetate	167.4	229.8
a,a'-dibromo-m-xylene	350.2	297.5
a,a'-dibromo-o-xylene	368.2	297.5
a,a'-dichloro-m-xylene	307.2	270.7
a,a'-dichloro-o-xylene	328.2	270.7
a,a'-dichloro-p-xylene	373.2	270.7
a-alanyl-a-alanine (DL)	483.2	458.5
acebutolol	394.2	420.4
acenaphthene	366.6	336.7
acenaphthylene	362.0	300.7
acetaldehyde	242.9	175.7
acetamide	353.0	323.3
acetanilide	387.5	374.0
acetohexamide	461.2	398.1
acetone	176.6	199.6
acetonitile	229.3	186.7
acetylacetone enol	254.8	245.8
acetylene	192.4	200.8
a-chloroacetic acid	334.3	295.3
a-chloroacetic acid	334.4	295.3
acridine	383.2	393.1
acrylamide	358.0	337.3
acrylic acid	285.5	364.3
acrylonitrile	189.6	211.0
a-D-glucopyranose (a-D-glucose)	423.2	453.0
a-D-glucose	414.0	453.0
adipic acid	426.4	376.1
alanylglycine (with decomp)	508.0	453.8
Albendazole	482.2	460.9
Aldicarb	372.2	353.7
Aldoxycarb	414.2	454.7
allobarbitiol	442.6	389.0
a-methylacrylic acid	287.5	301.8
a-methylstyrene	250.8	200.5
Ametryn	358.2	379.3
Aminocarb	367.2	344.6
amobarbital	429.2	418.5
a-naphthol	369.0	335.5
a-naphthyl acetate	319.2	394.1

androstanolone	454.0	441.7
Anilazine	433.2	464.0
aniline	267.1	294.9
anisaldazine	442.0	442.0
anthracene	488.9	431.0
anthraquinone	558.0	604.4
aprobarbital	414.2	385.3
atenolol	420.2	418.5
Atrazine	448.2	399.1
azelaic acid	380.0	381.2
Azimsulfuron	443.2	523.7
azoxybenzene	309.2	309.2
azulene	373.5	295.2
b(4-chlorophenoxy)-a-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	377.8	413.5
b-alanyl-b-alanine	480.1	458.5
barbital	462.6	500.8
beclomethasone-17,21-dipropionate	393.2	421.0
Bendiocarb	403.2	443.6
bendroflumethiazide	495.2	520.8
Benfluralin	339.2	365.1
benzaldehyde	216.0	293.0
benzamide	402.3	399.6
benzanilide	436.5	431.4
benzene	278.7	324.4
benzene-hexa-n-hexanoate	368.7	351.0
benzidine	400.2	565.0
benzil	368.0	420.3
benzimidazole	443.2	428.6
benzo[c]cinnoline	432.2	366.9
benzofluoranthene	424.0	348.9
benzoic acid	395.5	434.7
benzoic anhydride	313.2	265.6
benzonitrile	260.3	308.9
benzophenone	324.2	328.8
benzothiazole	275.6	277.6
benzothiophene	304.5	261.6
benzotrichloride	236.0	288.6
benzotrifluoride	244.0	179.4
benzoxazole	302.5	247.5
benzthiazide	508.2	508.2
benzyl alcohol	257.6	268.1
benzyl benzoate	293.1	344.6
benzylbromide	271.8	258.0
benzyliodide	299.5	293.6
benzylmethylsulfone	400.5	381.4
betamethasone	503.0	520.9
betamethasone-17-valerate	456.0	431.6
beta-sitosterol	413.3	358.6
betaxolol	344.2	346.9
biphenyl	341.5	382.5
bis(2-cyanoethyl)-N-nitroamine	327.0	382.0
bis-(4-aminophenyl)methane	363.7	405.8
bis(4-chlorophenyl)acetic acid	440.2	450.3

bis-[3,5-di-tert-butyl-4-hydroxybenzyl]sulfide	417.2	409.6
bis-hydroxyethylpiperazine	405.0	341.7
bisoprolol	373.2	318.0
bromobenzene	242.4	261.0
bromocyclohexane	216.9	225.0
bromomethane	179.5	128.6
bromotrichloromethane	267.5	242.6
butabarbital	438.2	420.4
Butacarb	376.2	430.1
butalbital	412.2	386.7
butanal	176.8	202.2
butane	134.9	164.2
butanoic acid	264.7	273.7
Butocarboxim	298.2	295.5
Butoxycarboxim	360.2	381.7
butyl 4-aminobenzoate	331.1	342.7
butyl 9-hydroxy-9H-fluorene-9-carboxylate	343.9	323.1
butyl acrylate	209.5	259.4
butyl alcohol	183.9	244.2
Butyl benzyl phthalate	238.2	359.2
butyl butanoate	181.7	236.8
butyl ethyl sulfide	178.1	228.0
butyl octadecanoate	299.7	317.4
caffeine	512.0	526.5
Carbaryl	418.2	383.8
carbazole	516.0	490.2
Carbendazim	523.2	474.9
carbon tetrabromide	363.2	421.1
carbon tetrachloride	249.0	309.6
carbon tetrafluoride	89.6	62.0
carbutamide	417.2	412.8
carvedilol	388.2	441.3
chlorbromuron	369.2	378.7
Chlorimuron	454.2	445.8
chlorobenzene	227.9	238.7
chlorocyclohexane	229.3	213.7
chlorocyclopentane	180.0	202.1
chlorodifluoromethane	115.7	56.1
chloroethane	134.8	171.2
chloroethyl methacrylate	235.1	259.8
chloropentafluorobenzene	257.5	241.2
chlorothiazide	616.2	610.5
chlorotoluron	421.2	414.5
chlorotrifluoroethylene	115.0	113.1
chloroxuron	424.2	426.6
chlorpropamide	400.2	366.3
chlorsulfuron	449.2	406.5
cholesterol acetate	388.0	354.0
cholesterol benzoate*	419.0	402.3
cholesterol*	421.0	376.7
chroman	269.8	314.0
chromone	330.3	369.9
chrysene	531.4	454.8

cinnamic acid	406.2	428.2
cinnamic anhydride	321.2	359.1
cinnamyl alcohol	308.2	268.4
cis,cis-1,3,5-tri-tert-butylcyclohexane	393.2	403.9
cis,trans-1,3,5-tri-tert-butylcyclohexane	338.2	403.9
cis-1,2-cyclohexanediol	371.6	269.8
cis-1,2-dimethylcyclohexane	223.3	175.6
cis-1,2-dimethylcyclopentane	219.4	159.7
cis-1,3-dimethylcyclohexane	197.6	175.6
cis-1,4-dimethylcyclohexane	185.7	175.6
cis-1,4-di-tert-butylcyclohexane	293.2	271.9
cis-2-butene	134.3	116.2
cis-2-hexene	132.0	134.5
cis-2-pentene	121.8	100.4
cis-3-chloro-2-butenoic acid	333.7	347.2
cis-6-octadecenoic acid	303.7	319.9
cis-9-octadecenoic acid	286.5	319.9
cis-crotonic acid	344.4	323.9
coronene	710.5	720.7
cortisone	495.0	556.7
cortisone acetate	509.0	493.5
coumarin	342.1	358.5
cyanamide	317.2	317.2
Cyanazine	440.2	491.3
cyanoacetamide	387.3	393.1
cyanocyclohexane	285.1	244.7
cyanogen	245.3	245.3
Cycloate	284.7	283.8
cyclobutane	182.4	210.6
cycloheptane	265.1	205.1
cycloheptanol	280.3	239.6
cycloheptatriene	198.0	201.1
cycloheptene	217.0	204.0
cyclohexane	279.8	193.8
cyclohexanethiol	189.6	185.9
cyclohexanol	297.0	231.8
cyclohexanone	245.2	232.7
cyclohexanone oxime	273.4	273.4
cyclohexene	169.7	191.3
cyclohexylbenzene	280.5	272.4
cycloocta-1,5-diene	204.0	214.3
cyclooctane	288.0	214.5
cyclooctanol	295.0	246.0
cyclooctatetraene	268.5	319.0
cyclooctene	259.2	214.4
cyclopentadiene	176.6	191.4
cyclopentane	179.7	179.9
cyclopentanethiol	155.4	171.1
cyclopentanol	257.4	222.2
cyclopentene	138.1	175.3
cyclopentyl methyl sulfide	169.9	201.7
cyclopentylamine	190.4	253.2
cyclopropane	145.6	198.9

cyclopropylamine	237.8	265.2
Cyprazine	440.2	440.2
D mannitol	439.1	403.5
D sorbitol	366.5	403.5
Dacthal	428.2	356.1
Daimuron	476.2	481.1
decachlorobiphenyl	577.7	649.8
decacyclene	666.0	635.4
decanal	268.2	285.2
decanoic acid	304.5	326.6
decyl methacrylate	250.7	290.1
deoxycorticosterone	414.0	475.7
deoxycorticosterone acetate	430.0	402.6
Desmetryn	358.2	340.4
desoxycorticosterone pivalate	476.2	476.2
dexamethasone	539.0	520.9
Diallate	298.2	239.3
diaminoethane	284.2	247.2
dibenzo[c,e][1,2]dithiin	386.2	411.6
dibenzodioxin	395.7	435.9
dibenzofuran	355.7	341.2
dibenzothiophene	371.0	375.3
dibromodichloromethane	294.4	242.6
dibromodifluoroethylene	162.8	195.2
Dibutyl phthalate	238.2	336.6
dichloroacetic acid	286.5	345.3
dichloromethane	178.2	192.7
dicyanomethane	305.0	285.5
dienestrol	500.2	435.8
diethyl disulfide	171.6	208.5
diethyl ether	156.9	169.7
diethyl o-phthalate	269.9	314.3
Diethyl phthalate	270.2	314.3
diethyl sulfide	169.2	188.9
diethyl terephthalate	317.2	314.3
diethylstilbestrol	442.0	382.3
Difenoxuron	412.2	422.8
diflubenzuron	512.2	452.6
difluoromethane	136.4	119.9
dihydroxyethane	260.6	284.4
diiodomethane	279.2	302.0
diisopropyl ketone	204.8	175.9
diisopropyl sulfide	195.1	137.7
Dimepiperate	312.2	339.5
Dimetan	318.7	324.1
Dimethametryn	338.2	331.7
dimethoxymethane	168.0	148.4
dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate	384.0	384.0
dimethyl amine	181.0	164.7
dimethyl ether	131.7	101.8
dimethyl fumarate	375.0	290.5
dimethyl maleate	254.0	290.5
dimethyl oxalate	327.6	455.9

Dimethyl phthalate	275.2	295.9
dimethyl sulfide	174.9	126.7
dimethyl sulfoxide	291.7	291.7
dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate	431.7	356.1
dimethylaminoethyl methacrylate	237.7	247.3
dimethyldisulfide	188.4	145.0
dimethylsulfone	382.0	328.7
di-n-butyl succinate	244.1	270.4
di-n-butyl sulfide	198.1	254.8
diphenyl ether	300.0	275.9
Diphenyl phthalate	345.2	407.5
diphenyl sulfone	398.2	388.2
diphenylacetic acid	420.4	414.4
diphenylacetylene	334.0	401.6
diphenylamine	326.2	367.1
diphenylcarbinol	338.5	331.6
diphenylmethane	298.3	283.4
diphenylsulfide	258.0	265.7
Dipropalin	353.2	381.3
Dipropetryn	378.2	331.7
dipropyl disulfide	187.7	231.5
dipropyl sulfide	170.4	228.0
diuron	432.2	418.2
DL 3,6-dimethyl-1,4-dioxane-2,5-dione	397.5	399.1
DL lactic acid	289.9	322.4
d-limonene	199.2	242.9
dodecane	263.6	283.5
dodecanedioic acid	402.5	384.5
dodecanoic acid	316.9	335.5
dodecanol	300.2	318.3
dotriacontane	343.5	338.9
dromostanolone propionate	399.2	395.7
dulcitol	460.3	403.5
d-valerolactone	263.0	240.7
dydrogesterone	442.2	397.7
E-3-chloro-2-butenoic acid	333.7	371.3
e-caprolactam	343.3	338.8
e-caprolactone	272.0	248.0
eicosanoic acid	348.2	349.4
esmolol	323.2	329.6
estradiol	452.0	471.0
estradiol-17-cypionate	424.2	441.2
estriol	555.0	525.9
estrone	533.2	455.1
Ethalfluralin	332.2	343.9
ethane	89.5	140.0
ethanethioamide	385.7	385.7
ethanoic acid	298.7	297.2
ethanol	158.8	198.4
Ethiofencarb	306.6	327.9
ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate	394.1	476.2
ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate	310.4	363.2
ethyl 4-aminobenzoate	362.8	329.8

ethyl acetate	189.3	196.3
ethyl carbamate	321.9	329.5
ethyl cyanoacetate	246.8	247.3
ethyl docosanoate	321.0	323.1
ethyl dodecanoate	271.5	282.5
ethyl eicosanoate	396.7	317.4
ethyl hexaconsanate	322.7	332.5
ethyl hexadecanoate	296.4	303.0
ethyl mercaptan	195.3	131.1
ethyl methyl sulfide	167.2	161.8
ethyl N-benzoyl-n-(3,4-dichlorophenyl)-dl-alaninate	341.7	347.0
ethyl nitrate	178.6	174.4
ethyl phenyl carbamate	326.0	340.9
ethyl propyl ether	145.7	193.2
ethyl propyl sulfide	156.1	210.4
ethyl tetracosanate	327.4	336.3
ethyl triacontanoate	341.5	339.7
ethyl(1,1-dimethylpropyl)malononitrile	307.5	312.4
ethylbenzene	178.2	203.8
ethylcyclohexane	161.4	214.6
ethylcyclopentane	134.7	203.7
ethylene	104.0	67.6
ethylene carbonate	309.5	269.2
ethylene oxalate	415.0	286.7
ethylene oxide	160.7	202.9
ethylestrenol	350.2	395.4
ethylmethylsulfone	307.7	303.2
ethynodiol diacetate	399.2	398.3
ethynyl estradiol	456.2	349.8
Fenobucarb	304.7	327.2
Fenothiocarb	313.7	332.1
fenuron	406.2	386.4
Flazasulfuron	441.2	442.3
Flufenoxuron	444.2	461.6
flumethiazide	573.2	578.7
fluocinolone acetonide	539.2	591.8
fluocinonide	583.2	522.5
fluometuron	437.2	377.7
fluorene	387.9	350.5
fluorobenzene	230.9	216.0
fluorometholone	568.2	518.6
fluorotrichloromethane	162.7	178.1
flurandrenolide	523.2	592.4
Forchlorfenuron	440.2	490.4
furan	187.6	181.7
furfural	235.1	246.6
furfuryl alcohol	258.6	240.2
glutaric acid	371.0	373.7
glyburide	442.2	465.6
glyceryl triacetate	275.3	278.2
glyceryl trilaurate	319.5	344.4
glyceryl trimyristate	330.2	351.1
glyceryl tripalmitate	338.9	356.4

glyceryl tristearate	345.7	360.7
Halosulfuron	449.2	419.5
heptabarbital	447.2	472.0
heptadecanoic acid	334.3	342.5
heptanal	229.3	254.7
heptane	182.6	229.7
heptanoic acid	265.8	307.2
hexachlorobenzene	505.0	534.5
hexachlorocyclopropane	376.0	406.1
hexachloroethane	458.0	461.3
hexacontane	373.2	365.1
hexadecane	291.1	292.2
hexadecanoic acid	335.7	339.8
Hexaflumuron	476.7	451.7
hexafluoroacetone	147.7	122.5
hexafluorobenzene	278.3	328.9
hexafluoroethane	173.1	210.6
hexamethylbenzene	438.7	486.1
hexanal	243.2	240.6
hexanamide	374.0	338.0
hexatriacontane	349.2	344.8
hexyl ethanoate	212.1	262.5
hexyl N-phenylcarbamate	328.0	359.3
hydrazobenzene (1,2-diphenylhydrazine)	407.2	402.9
hydrochlorothiazide	547.2	592.2
hydrocinnamic acid	321.2	327.2
hydrocortisone	485.0	571.6
hydrocortisone 21-heptanoate	384.2	444.2
hydrocortisone 21-hexanoate	388.2	447.7
hydrocortisone-17-butyrate	395.0	468.8
hydrocortisone-21-acetate	497.0	505.7
hydrocortisone-21-butyrate	463.2	456.7
hydrocortisone-21-propionate	484.2	462.6
hydrocortisone-21-valerate	457.2	451.8
hydroflumethiazide	543.7	560.4
Imazosulfuron	456.2	502.7
imidazole	361.9	308.7
indene	271.7	242.2
iodobenzene	241.8	282.8
iodomethane	206.8	204.1
Ipazine	360.2	340.6
isobutane	113.7	117.7
isobutene	132.4	139.7
isobutyl alcohol	171.2	195.4
isobutyl mercaptan	128.3	136.8
isochroman	277.5	314.0
isonicotinic acid	593.0	452.8
Isoprocarb	367.2	319.8
isopropyl 4,4'-dibromobenzilate	348.1	367.5
isopropyl ether	187.8	118.5
isopropyl methyl ketone	180.0	182.3
isopropyl methyl sulfide	171.7	132.9

isopropyl nitrate	190.9	209.9
isopropyl phenylcarbamate	359.5	313.5
isopropyl-3-chlorophenylcarbamate	313.9	327.8
isopropylbenzene	177.1	210.1
Isoproturon	431.2	371.1
isoquinoline	299.6	277.3
Isouron	392.7	414.0
L-carvone	247.7	335.7
levulinic acid	306.2	304.1
L-iditol	352.8	403.5
linoelaidic acid	303.0	295.6
linuron	367.2	365.0
Lufenuron	439.2	469.1
lynestrenol	432.2	358.1
m-(methylamino)benzoic acid	402.2	428.9
m-acetamidobenzoic acid	523.2	510.3
m-acetotoluidide	339.2	387.8
m-acetoxybenzoic acid	404.2	419.3
maleic anhydride	325.7	293.5
malonamide	443.0	486.9
m-alpha-bromotolunitrile	366.2	335.0
m-aminoacetanilide	361.2	435.3
m-aminobenzaldehyde	303.2	329.6
m-aminobenzamide	384.2	469.9
m-aminobenzyl alcohol	370.2	333.5
m-aminophenol	399.0	335.1
m-benzenedicarboxylic acid	621.2	653.9
m-bromoacetanilide	361.2	409.2
m-bromoacetophenone	281.2	314.5
m-bromoaniline	291.2	301.3
m-bromobenzamide	428.2	439.9
m-bromobenzoic acid	428.2	425.0
m-bromobenzonitrile	311.2	313.7
m-bromobenzyl bromide	314.2	295.5
m-bromomethylbenzoic acid	429.2	438.7
m-bromophenol	306.2	305.2
m-bromophenyl urea	438.2	464.8
m-bromotoluene	233.2	246.8
m-chloroacetanilide	352.2	392.0
m-chloroaniline	263.2	281.5
m-chlorobenzaldehyde	291.2	279.9
m-chlorobenzamide	407.2	420.2
m-chlorobenzonitrile	314.2	293.9
m-chlorobenzyl bromide	295.2	277.2
m-chloroethylbenzene	210.6	223.0
m-chlorotoluene	225.2	227.1
m-cyanoaniline	326.2	343.6
m-cyanobenzaldehyde	351.2	342.0
m-cyanobenzoic acid	490.2	467.4
m-cymene	209.5	224.8
m-diacetylbenzene	305.2	333.0
m-diethylbenzene	189.3	202.2

m-diethynylbenzene	276.2	334.7
Mebendazole	561.7	495.8
mestanolone	465.2	421.9
Methabenzthiazuron	393.2	491.4
methacrylamide	385.1	316.7
methandienone	436.2	369.2
methanethiol	150.2	88.2
methanol	175.3	225.6
Methiocarb	393.2	364.7
Methomyl	351.2	351.9
m-ethoxyacetanilide	369.2	391.8
m-ethoxybenzamide	412.2	413.6
methoxybenzene	293.2	249.4
m-ethoxybenzoic acid	410.2	426.4
m-ethoxyphenyl acetate	307.2	293.4
methyclothiazide	498.2	518.6
methyl 2-(2,4,5-trichlorophenoxy)acetate	361.9	313.4
methyl 2-(2,4,5-trichlorophenoxy)butyrate	316.5	325.6
methyl 2-(2,4,5-trichlorophenoxy)propionate	360.6	318.1
methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	314.4	354.8
methyl 2,4-dichlorophenoxyacetate	315.4	299.1
methyl 3,6-dichloro-2-methoxybenzoate	304.6	321.3
methyl 3-m-tolylcarbamoyloxyphenylcarbamate	423.8	493.3
methyl 4-(2,4-dichlorophenoxy)butyrate	309.6	316.2
methyl 4-amino-3,5,6-trichloro-2-picolinate	394.3	382.0
methyl 4-aminobenzoate	385.1	320.8
methyl 4-hydroxybenzoate	398.5	324.2
methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	358.3	369.9
methyl acetate	174.9	168.3
methyl acrylate	197.5	205.3
methyl a-D-mannopyranoside	455.2	388.0
methyl benzoate	261.0	259.6
methyl butyl sulfide	175.6	210.4
methyl carbamate	328.6	319.9
methyl chloride	174.5	181.6
m-ethyl cyanobenzoate	329.2	383.0
methyl docosanoate	325.0	320.4
m-ethyl hydroxybenzoate	346.2	332.8
methyl isopropyl ether	127.3	111.2
methyl methacrylate	225.0	187.4
methyl myristate	291.6	288.4
methyl n-butyl ether	157.5	193.2
methyl n-decyl ether	243.5	271.7
methyl nitrate	190.2	184.1
m-ethyl nitrobenzoate	320.2	328.6
m-ethyl nitrocinnamate	352.2	368.9
methyl N-phenylcarbamate	325.0	329.3
methyl octadecanoate	310.9	307.1
methyl palmitate	307.2	298.6
methyl perfluorobutanoate	191.4	224.9
methyl p-N,N-dimethylaminobenzoate	371.8	272.4
methyl propyl ether	134.0	169.7
methyl propyl sulfide	160.2	188.9

methyl tert-butyl ether	164.6	196.1
methyl tert-butyl sulfide	190.8	220.9
methyl tetrachloroterephthalic acid ester	444.3	427.7
methyl-3,4-dichlorophenylcarbamate	381.4	361.1
methylamine	179.7	191.1
m-ethylbenzoic acid	320.2	384.5
methylcyclobutane	138.6	151.0
methylcyclohexane	146.6	184.7
methylcyclopentane	130.7	169.8
Methyldymron	345.2	452.3
methylenecyclobutane	138.5	158.4
methylhydrazine	220.8	214.4
m-ethylphenol	269.2	272.9
methylphenylsulfide	256.4	241.0
methylphosphonyl chlorofluoride	250.7	250.7
methylphosphonyl dichloride	306.1	306.1
methylphosphonyl difluoride	236.3	236.3
methylprednisolone	513.2	529.8
methylprednisolone-21-acetate	498.2	471.1
methyltestosterone acetate	448.0	429.8
methyltestosterone propionate	418.0	388.0
m-ethyltoluene	177.2	218.6
metobromuron	369.2	364.4
Metolcarb	349.7	341.5
metoprolol	308.2	318.5
Metoxuron	399.7	414.6
m-fluorobenzoic acid	397.2	385.1
m-hydroxyacetanilide	422.2	438.7
m-hydroxyacetophenone	369.2	348.3
m-hydroxybenzaldehyde	381.2	333.5
m-hydroxybenzaldehyde oxime	363.2	380.7
m-hydroxybenzamide	440.2	473.8
m-hydroxybenzyl alcohol	346.2	337.1
m-hydroxytoluene	285.4	280.7
m-iodoacetanilide	392.2	426.0
m-iodoaniline	298.2	320.6
m-iodobenzaldehyde	330.2	318.9
m-iodobenzaldehyde oxime	335.2	367.2
m-iodobenzamide	459.2	459.2
m-iodobenzyl bromide	324.2	313.5
m-iodophenol	313.2	324.5
m-iodophenyl acetate	311.2	302.2
m-iodotoluene	246.0	266.2
m-isopropylbenzoic acid	324.2	390.8
m-methoxyacetanilide	353.2	390.9
m-methoxyacetophenone	368.2	306.1
m-methoxyaniline	261.2	314.8
m-methoxybenzaldoxime	313.2	337.1
m-methoxybenzoic acid	383.2	430.1
m-methoxyphenyl acetate	312.2	281.3
m-methyl aminobenzoate	311.2	320.8
m-methyl bromobenzoate	305.2	294.7
m-methyl chlorobenzoate	294.2	277.5

m-methyl cyanobenzoate	338.2	331.6
m-methyl hydroxybenzoate	343.2	324.2
m-methyl iodobenzoate	327.2	311.6
m-methyl nitrobenzoate	352.2	319.5
m-methyl nitrocinnamate	397.2	365.4
m-N,N'-diacetylphenylenediamide	464.2	444.5
m-nitroacetanilide	428.2	433.9
m-nitroacetophenone	354.2	342.8
m-nitrobenzaldehyde	331.2	328.0
m-nitrobenzaldoxime	395.2	375.6
m-nitrobenzamide	415.2	468.3
m-nitrobenzoic acid	414.3	453.4
m-nitrobenzonitrile	391.2	342.0
m-nitrobenzoyl chloride	308.2	319.4
m-nitrobenzyl alcohol	300.2	332.0
m-nitrobenzyl bromide	332.2	322.0
m-nitrobenzyl chloride	319.2	306.7
m-nitrobenzyl cyanide	335.2	348.4
m-nitrobenzyl iodide	359.2	357.6
m-nitrobromobenzene	329.2	299.7
m-nitroiodobenzene	311.2	319.0
m-nitrophenentole	307.2	323.8
m-nitrophenol	371.2	333.6
m-nitrophenyl acetate	329.2	310.1
m-nitrophenylacetic acid	393.2	392.5
m-N-methylnitroaniline	341.2	343.0
m-n-propylbenzoic acid	316.2	386.3
mono(2,2-dimethylhydrazide) butanedioic acid	431.4	418.0
Monuron	443.7	402.3
m-phenylenediacetic acid	443.2	418.5
m-phenylenediamine	335.5	374.3
m-propylphenol	299.2	288.2
m-terphenyl	360.0	450.1
m-tolualdehyde oxime	333.2	326.4
m-toluamide	368.2	415.4
m-toluic acid	381.9	400.5
m-toluidine	241.7	276.8
m-tolunitrile	250.2	289.2
m-tolylurea	415.2	443.5
m-xylene	225.3	251.3
myo-inositol	496.9	421.8
N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine	327.5	297.3
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine	318.4	390.2
N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine	372.1	390.1
N-(3,4-dichlorophenyl)-2-methyl-2-propenamide	395.5	371.2
N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea	399.2	414.6
N-(3-chloro-4-methylphenyl)-2-methylpentanamide	353.2	378.9
N-(4-chlorophenyl)-2,2-dimethylpentanamide	360.2	388.1
N'-(4-chlorophenyl)-N-methoxy-N-methylurea	353.4	350.7
N-(cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl)benzenamine	305.8	297.5
N,N'-(2-hydroxyethyl)-1,4-diaminoanthraquinone	521.2	533.1
N,N-(2-hydroxyethyl)-4-(4-nitrophenyl)azoaniline	484.2	431.3
N,N-(2-hydroxyethyl)-4-phenylazoaniline	407.0	428.4

N,N-diethyl-2-(1-naphthyloxy)propionamide	345.3	351.2
N,N-dimethyl-1,3-propanediamine	194.4	246.3
N,N-dimethyl-2,2-diphenylacetamide	407.1	322.7
N,N-dimethyl-2,2-diphenylbenzeneacetamide	402.0	390.0
N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide	372.2	373.2
N,N-dimethyl-4-phenylazoaniline	389.2	323.1
N,N-dimethylaniline	275.6	228.7
N,N-dimethylformamide	212.9	212.9
N,N'-dimethylhydrazine	264.3	269.2
N,N-dimethylhydrazine	216.0	216.0
N,N'-dimethyl-N,N'dinitro-1,2-ethanediamine	410.0	355.3
N,N'-dimethyl-N,N'dinitro-1,6-hexanediamine	331.0	368.1
N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea	434.1	426.4
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea	430.5	371.1
N,N'-di-n-hexyladipamide	432.0	388.9
N,N'-dinitro-diaminomethane	371.0	413.4
N,N'-dinitroethanediamine	450.0	412.0
N,N'-di-n-propyladipamide	452.0	385.1
N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	432.0	430.6
N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl-propanamide	370.2	430.7
N-[4-methyl-3-[[(trifluoromethyl)sulfonyl]amino]phenyl]acetamide	455.7	474.8
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea	435.3	431.5
N-acetyl-D-leucine amide	404.0	427.3
N-acetylglycine amide	408.2	454.0
N-acetylglycyl-L-prolinamide	457.8	478.4
N-acetyl-L-alanine amide	431.0	456.2
N-acetyl-L-isoleucinamide	529.6	427.3
N-acetyl-L-prolyl-glycinamide	434.1	478.4
N-acetyl-pyrazinamide	366.7	366.7
N-acetylsarcosinamide	412.7	363.3
N-allyl-N-phenylthiourea	375.0	375.0
nandrolone	385.2	395.1
nandrolone decanoate	308.2	382.6
naphthalene	353.4	339.3
naphthalene 1,8-disulfide	394.8	339.8
naphthalene 1,8-disulfide s-oxide	421.2	421.2
N-benzylaniline	305.6	345.9
N-butyl dodecanamide	322.1	340.0
n-butyl mercaptan	157.5	192.3
N-butyl tetradecanamide	336.1	345.3
n-butylbenzene	185.3	246.0
n-butylcyclohexane	198.4	244.7
n-butylcyclopentane	165.2	238.4
N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea	374.3	413.4
N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline	338.5	278.6
N-butylurea	369.3	371.6
n-decane	243.5	266.7
N-decyl hexadecanamide	347.0	359.4
n-decyl-a-cyanoacrylate	294.5	311.4
n-decylcyclohexane	271.4	303.9
n-decylcyclopentane	251.0	294.4
N-decylundecanamide	344.0	351.6

N-dimethylaminosuccinamic acid	431.4	431.4
n-docosane	316.1	316.2
n-dodecylcyclohexane	258.8	313.5
n-dononacontahectane	399.1	388.2
n-eicosane	309.7	309.5
neopentyl-4,4,4-trinitrobutyrate	333.5	361.4
n-ethyl-a-cyanoacrylate	243.2	231.0
N-ethylurea	365.1	364.8
n-hectane	388.5	378.2
n-heneicosane	313.7	313.0
n-heptacosane	332.1	329.3
n-heptadecane	295.1	297.1
N-heptylmyristamide	343.0	351.6
n-hexacosane	329.5	327.1
n-hexane	177.8	212.3
N-hexyl decanamide	311.0	340.0
N-hexyl hexadecanamide	343.1	353.4
N-hexyl tetradecanamide	334.0	349.6
nicosulfuron	415.2	410.9
nicotinic acid	510.0	400.8
N-isopropylcarbazole	395.2	348.6
N-isopropylurea	280.8	337.7
Nitralin	425.2	432.0
nitrobenzene	278.8	293.1
nitroethane	183.7	174.4
nitromethane	244.8	183.1
N-laurylnonanamide	341.0	351.6
N-methyl O-methyl O-2-chloro-4-tert-butylphenyl phosphoramidate	332.0	332.0
N-methyl-2,4,6,N-tetranitroaniline	402.6	507.7
N-methyl-2-chlorophenylcarbamic acid ester	362.7	345.2
N-methylacetamide	303.8	300.6
N-methylcarbazole	362.5	430.5
N-methyldiphenylacetamide	439.8	413.4
N-methyl-N-nitrobutanamine	331.0	283.8
N-methylpyrrole	216.9	271.0
N-methylurea	378.1	360.1
N-myristylheptanamide	334.0	351.6
N-nitro-bis(N,N-cyanomethyl) amine	367.0	378.1
N-nitro-N-methylaminomethane	327.0	232.6
n-nonacosane	336.6	333.5
n-octacosane	334.5	331.5
n-octane	216.4	244.1
n-octylbenzene	234.2	281.7
nonadecane	305.3	305.7
nonadecanoic acid	341.2	347.3
nonanal	253.9	276.5
nonane	219.7	256.3
nonanoic acid	285.5	321.1
nonyl acrylate	236.5	303.8
nonyl phenylcarbamate	327.0	362.8
norethindrone	479.0	397.1
norethindrone acetate	480.0	426.2
norgestrel	482.2	456.1

Novaluron	450.7	440.3
N-palmitoyl-pyrazinamide	362.7	381.7
n-pentacontane	366.9	358.8
n-pentacosane	326.7	324.6
n-pentadecane	283.1	286.8
n-pentatriacontane	347.2	343.5
N-phenyl-N[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)	357.2	454.7
n-propylbenzene	173.6	227.5
n-propylcyclohexane	178.3	231.0
N-propylstearamide	354.0	351.6
N-propylurea	381.0	368.6
N-salicylidene-m-aminobenzoic acid	464.0	509.0
N-stearylpropanamide	350.0	351.6
N-Sulfanilylsulfanilamide	407.2	447.0
N-tert-butylurea	449.8	447.8
n-tetracosane	324.1	322.0
n-tetratetracontane	360.9	353.8
n-tricosane	320.7	319.2
n-tridecane	267.8	274.1
n-undecane	247.6	275.7
N-vinylpyrrolidone	286.2	286.2
O-(2,4-dichlorophenyl) O-methyl-(1-methylethyl) phosphoramidothioate	321.5	321.5
O-(2-chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate	323.9	315.1
O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate	325.3	309.4
O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphonothioate	345.6	344.2
o-(methylamino)benzoic acid	452.2	405.0
O,O,O',O'-tetramethyl O,O'-thiodi-p-phenylene bis(phosphorothioate)	303.2	298.9
O,O-diethyl O-4-nitrophenyl phosphorothioate	278.1	317.7
O,O-diethyl O-quinoxalin-2-yl phosphothioate	304.1	338.2
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl) phosphate	312.5	300.9
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	315.0	323.2
O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate	310.4	321.8
O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	313.0	295.0
O,O-dimethyl O-(4-aminosulfonylphenyl)phosphorothioate	344.2	282.1
O,O-dimethyl O-4-nitrophenyl phosphorothioate	308.2	300.1
O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate	321.0	306.1
O,O-dimethyl S-phthalimidomethyl phosphorodithioate	343.2	343.2
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate	318.7	306.7
O,S-dimethyl phosphoroamidothioate	316.8	316.8
O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl O,O-diethyl phosphorothioate	324.4	353.1
o-acetamidobenzoic acid	458.2	467.9
o-acetotoluidide	385.2	387.8
o-acetoxybenzoic acid	408.2	396.8
o-alpha-bromotolunitrile	346.2	335.0
o-aminoacetanilide	405.2	417.4
o-aminoacetophenone	293.2	318.5
o-aminobenzaldehyde	313.2	277.8
o-aminobenzaldehyde oxime	408.2	377.1
o-aminobenzyl alcohol	355.2	285.3
o-aminophenol	447.4	327.5
o-benzenedicarboxylic acid	507.2	624.9
o-bromoacetanilide	372.2	405.8

o-bromoaniline	305.2	297.5
o-bromoanisole	275.7	286.9
o-bromobenzaldehyde	295.2	295.8
o-bromobenzamide	428.2	414.0
o-bromobenzoic acid	423.2	399.1
o-bromobenzonitrile	326.2	313.7
o-bromobenzyl alcohol	353.2	281.5
o-bromobenzyl bromide	304.2	295.5
o-bromomethylbenzoic acid	423.2	438.7
o-bromophenol	278.2	301.4
o-bromophenyl urea	475.2	450.3
o-bromotoluene	245.2	246.8
o-chloroacetanilide	361.2	388.6
o-chloroaniline	274.2	277.7
o-chloroanisole	246.4	268.6
o-chlorobenzaldehyde	284.2	276.1
o-chlorobenzamide	414.2	394.3
o-chlorobenzonitrile	316.2	293.9
o-chlorobenzyl alcohol	347.2	263.1
o-chloroethylbenzene	190.5	223.0
o-chlorotoluene	235.2	227.1
octadecanamide	377.2	363.0
octadecane	301.3	301.6
octadecanoic acid	342.5	345.0
octadecanol	334.2	325.4
octafluoropropane	125.5	190.7
octafluorotetrahydrothiophene	266.7	254.5
octanal	288.2	266.5
octanoic acid	289.7	314.7
octyl methacrylate	230.3	276.1
o-cyanoaniline	323.2	343.6
o-cyanobenzaldehyde	382.2	342.0
o-cyanobenzoic acid	463.2	467.4
o-cymene	201.7	224.8
o-diacetylbenzene	313.2	333.0
o-diethylbenzene	242.0	202.2
o-ethoxyacetanilide	352.2	389.2
o-ethoxybenzamide	405.2	393.6
o-ethoxybenzoic acid	292.2	405.2
o-ethoxyphenyl acetate	275.2	293.4
o-ethyl aminobenzoate	286.2	309.8
o-ethyl cyanobenzoate	343.2	383.0
o-ethyl nitrobenzoate	303.2	328.6
o-ethyl nitrocinnamate	317.2	368.9
O-ethyl O-(4-nitrophenyl)phenylphosphonothioate	308.2	309.4
o-ethylbenzoic acid	341.2	384.5
o-ethyltoluene	192.2	218.6
o-fluorobenzoic acid	400.2	359.2
o-hydroxyacetanilide	364.5	424.2
o-hydroxyacetophenone	277.2	322.4
o-hydroxybenzaldehyde	266.2	329.7
o-hydroxybenzaldehyde oxime	336.2	380.7
o-hydroxybenzamide	412.2	422.0

o-hydroxybenzyl alcohol	360.2	288.9
o-hydroxybiphenyl	330.6	368.7
o-hydroxytoluene	304.2	280.7
o-iodoacetanilide	383.2	422.7
o-iodoaniline	331.2	316.8
o-iodobenzaldehyde	310.2	315.1
o-iodobenzaldehyde oxime	381.2	367.2
o-iodobenzamide	457.2	433.3
o-iodobenzyl alcohol	363.2	299.5
o-iodobenzyl bromide	330.2	313.5
o-iodophenol	316.2	320.7
o-isopropylbenzoic acid	337.2	390.8
o-methoxyacetanilide	361.2	388.0
o-methoxyaniline	279.2	314.8
o-methoxybenzaldehyde	311.2	313.3
o-methoxybenzaldoxime	365.2	383.5
o-methoxybenzamide	402.2	392.8
o-methoxybenzoic acid	374.2	406.0
o-methoxyphenol	305.2	314.9
o-methoxyphenyl acetate	283.2	281.3
o-methyl aminobenzoate	297.2	298.3
o-methyl cyanobenzoate	324.2	331.6
o-methyl hydroxybenzoate	265.2	301.7
o-methyl nitrobenzoate	260.2	319.5
o-methyl nitrocinnamate	346.2	365.4
o-methylbenzyl alcohol	309.2	282.8
o-N,N'-diacetylphenylenediamide	459.2	420.2
o-nitroacetanilide	367.2	411.3
o-nitroacetophenone	301.2	342.8
o-nitrobenzaldehyde	317.2	302.1
o-nitrobenzaldoxime	376.2	375.6
o-nitrobenzamide	448.2	455.4
o-nitrobenzoic acid	419.0	440.6
o-nitrobenzonitrile	383.2	342.0
o-nitrobenzoyl chloride	293.2	319.4
o-nitrobenzyl alcohol	347.2	320.1
o-nitrobenzyl bromide	320.2	322.0
o-nitrobenzyl chloride	322.2	306.7
o-nitrobenzyl cyanide	357.2	348.4
o-nitrobenzyl iodide	348.2	357.6
o-nitrobromobenzene	315.2	299.7
o-nitroiodobenzene	327.2	319.0
o-nitrophenentole	275.3	323.8
o-nitrophenol	318.2	307.7
o-nitrophenyl acetate	314.2	310.1
o-nitrophenylacetic acid	416.2	392.5
o-nitrotoluene	269.2	275.2
o-N-methylhydroxyaniline	370.2	341.0
o-N-methylnitroaniline	310.2	318.9
o-N-methylphenylenediamine	295.2	344.5
o-n-propylbenzoic acid	331.2	386.3
o-phenylenediacetic acid	423.2	418.5
o-phenylenediamine	373.9	315.7

o-phenylenepyrene	435.2	355.9
Orbencarb	282.2	304.4
o-terphenyl	329.4	371.0
o-tolualdehyde oxime	322.2	326.4
o-toluamide	413.2	415.4
o-toluic acid	376.9	400.5
o-toluidine	287.6	276.8
o-tolunitrile	259.2	289.2
o-tolylurea	464.2	443.5
Oxamyl	374.2	373.2
oxandrolone	498.2	432.8
Oxasulfuron	431.2	491.9
o-xylene	247.8	251.3
oxymetholone	452.2	489.3
p-(methylamino)benzoic acid	441.2	428.9
p,p'-dichlorobenzophenone	420.0	375.3
p-acetamidobenzoic acid	524.2	510.3
p-acetotoluidide	427.2	387.8
p-a-cumylphenol	346.4	320.3
p-alpha-bromotolunitrile	389.2	335.0
p-aminoacetanilide	436.2	435.3
p-aminobenzaldehyde	345.2	372.4
p-aminobenzaldehyde oxime	397.2	377.1
p-aminobenzamide	387.2	469.9
p-aminobenzene sulphonamide	439.3	305.1
p-aminobenzyl alcohol	338.2	333.5
p-aminophenol	462.5	378.7
p-benzoquinone	388.0	421.0
p-bromoacetanilide	440.2	409.2
p-bromoacetophenone	324.2	314.5
p-bromoaniline	339.2	340.4
p-bromoanisole	286.2	286.9
p-bromobenzaldehyde	340.2	338.6
p-bromobenzamide	462.2	439.9
p-bromobenzoic acid	525.2	480.2
p-bromobenzonitrile	386.2	354.4
p-bromobenzyl alcohol	350.2	305.6
p-bromobenzyl bromide	336.2	295.5
p-bromoethynylbenzene	338.2	320.7
p-bromoisopropylbenzene	250.2	247.6
p-bromomethylbenzoic acid	502.2	438.7
p-bromophenetole	277.2	300.5
p-bromophenyl urea	500.2	464.8
p-bromotoluene	302.2	278.9
p-chloroacetanilide	452.2	392.0
p-chloroacetophenone	293.2	294.7
p-chloroaniline	344.2	318.1
p-chlorobenzaldehyde	320.2	316.2
p-chlorobenzamide	452.2	420.2
p-chlorobenzonitrile	369.2	332.1
p-chlorobenzyl alcohol	348.2	287.2
p-chlorobenzyl bromide	324.2	277.2
p-chlorobenzyl p-chlorophenyl sulfide	343.8	346.1

p-chlorophenetole	294.2	284.4
p-chlorotoluene	280.7	256.6
p-cyanoaniline	359.2	388.3
p-cyanobenzaldehyde	374.2	386.4
p-cyanobenzoic acid	492.2	528.1
p-cymene	199.2	224.8
p-diacetylbenzene	386.2	333.0
p-diethylbenzene	230.3	202.2
p-diethynylbenzene	368.2	384.7
p-difluorobenzene	260.2	248.8
p-dioxanone	301.7	269.7
Pebulate	251.2	282.8
penbutolol	343.2	410.1
Pencycuron	403.2	452.0
Pendimethalin	330.2	403.8
pentabromophenol	502.0	518.4
pentachloroaniline	505.8	402.5
pentachlorobenzene	357.7	331.7
pentachloronitrobenzene	418.0	362.3
pentachlorophenol	462.5	406.9
pentadecanoic acid	325.7	336.8
pentaerythritol	538.7	468.9
pentaerythritol tetrafluoride	249.4	265.5
pentaerythrityl tetrabromide	433.5	398.2
pentafluoroaniline	306.8	288.7
pentafluorobenzene	225.7	217.9
pentafluorochloroethane	173.7	142.3
pentafluoroethane	172.6	104.5
pentafluoronitrobenzene	250.5	261.6
pentafluorophenol	310.6	293.1
pentamethylbenzene	328.2	304.9
pentane	143.5	191.0
pentanoic acid	239.5	287.3
pentyl 4-aminobenzoate	325.1	347.6
perfluorotoluene	207.0	181.6
perylene	551.0	531.8
p-ethoxyacetanilide	407.2	391.8
p-ethoxyaniline	277.2	325.1
p-ethoxybenzamide	475.2	413.6
p-ethoxyphenylacetate	333.2	293.4
p-ethyl cyanobenzoate	327.2	383.0
p-ethyl hydroxybenzoate	389.2	332.8
p-ethyl methoxybenzoate	280.2	300.8
p-ethyl nitrobenzoate	330.2	328.6
p-ethyl nitrocinnamate	415.2	368.9
p-ethylphenol	320.2	272.9
p-ethyltoluene	211.2	218.6
p-fluorobenzoic acid	458.2	435.2
phenanthrene	372.4	375.0
phenanthridine	379.7	347.9
phenazine	450.2	472.7
phenobarbital	447.2	509.0
Phenobenzuron	392.2	410.6

phenol	314.0	299.3
phenolphthalein	534.0	624.3
phenoxathiin	328.8	413.4
phenyl glycidyl ether	279.8	326.4
phenyl vinyl sulfone	343.4	305.3
phenylacetic acid	349.9	332.6
phenylacetylene	228.0	275.1
phenylaminoethyl methacrylate	297.5	337.8
phenylhydrazine	292.8	298.8
phenyl-o-tolylmethane	279.8	297.2
phenylurea	420.6	429.7
phthalazine	364.5	287.1
phthalic anhydride	403.3	375.7
p-hydroxyacetanilide	441.2	438.7
p-hydroxyacetophenone	382.2	348.3
p-hydroxybenzaldehyde	389.2	376.8
p-hydroxybenzaldehyde oxime	345.2	380.7
p-hydroxybenzamide	435.2	473.8
p-hydroxybenzyl alcohol	398.2	337.1
p-hydroxytoluene	307.9	317.2
picene	637.2	534.5
picolinic acid	411.0	400.8
picric acid	394.1	419.2
pimilic acid	377.5	378.1
pindolol	442.2	426.1
p-iodoacetanilide	457.2	426.0
p-iodoacetophenone	358.2	333.8
p-iodoaniline	336.2	362.3
p-iodoanisole	325.2	304.9
p-iodobenzaldehyde	351.2	360.4
p-iodobenzamide	491.2	459.2
p-iodobenzyl alcohol	345.2	323.6
p-iodobenzyl bromide	353.2	313.5
p-iodophenetole	302.2	316.4
p-iodophenol	367.2	366.7
p-iodophenyl acetate	305.2	302.2
p-iodotoluene	306.7	300.7
piperidine	262.1	208.3
Pirimicarb	363.7	311.2
p-isopropylbenzoic acid	391.2	390.8
pivaldehyde	272.1	225.1
p-methacryloyloxybenzoic acid	455.0	398.0
p-methoxyacetanilide	400.3	390.9
p-methoxyacetophenone	312.2	306.1
p-methoxyaniline	330.2	314.8
p-methoxybenzaldehyde	275.2	313.3
p-methoxybenzaldoxime	405.2	383.5
p-methoxybenzamide	436.2	415.4
p-methoxyphenol	329.2	318.5
p-methoxyphenyl acetate	327.2	281.3
p-methyl bromobenzoate	354.2	294.7
p-methyl chlorobenzoate	317.2	277.5
p-methyl cyanobenzoate	335.2	331.6

p-methyl iodobenzoate	387.2	311.6
p-methyl methoxybenzoate	322.2	287.3
p-methyl nitrobenzoate	369.2	319.5
p-methyl nitrocinnamate	434.2	365.4
p-methyl toluate	307.2	273.4
p-methylacetophenone	301.2	223.9
p-methylbenzyl alcohol	333.2	282.8
p-N,N'-diacetylphenylenediamide	577.2	444.5
p-n-hexyloxybenzylideneaniline	321.6	324.9
p-nitroacetanilide	489.2	433.9
p-nitroacetophenone	354.2	342.8
p-nitrobenzaldehyde	379.2	370.6
p-nitrobenzaldoxime	406.2	375.6
p-nitrobenzamide	473.2	468.3
p-nitrobenzoic acid	512.4	512.3
p-nitrobenzonitrile	422.2	386.5
p-nitrobenzoyl chloride	348.2	319.4
p-nitrobenzyl alcohol	366.2	332.0
p-nitrobenzyl bromide	373.2	322.0
p-nitrobenzyl chloride	344.2	306.7
p-nitrobenzyl cyanide	390.2	348.4
p-nitrobenzyl iodide	400.2	357.6
p-nitrobromobenzene	400.2	338.6
p-nitroiodobenzene	447.2	360.5
p-nitrophenentole	333.2	323.8
p-nitrophenol	388.2	376.9
p-nitrophenyl acetate	356.2	310.1
p-nitrophenylacetic acid	426.2	392.5
p-N-methylhydroxyaniline	360.2	348.1
p-N-methylnitroaniline	425.2	343.0
p-N-methylphenylenediamine	309.2	344.5
polythiazide	475.7	473.3
p-phenylazoaniline	398.2	436.4
p-phenylenediacetic acid	517.2	418.5
p-phenylenediamine	412.3	430.2
p-propylphenol	294.2	288.2
p-quaterphenyl	587.2	652.2
prasterone	423.0	420.8
prasterone acetate	440.2	431.4
prasterone butyrate	436.2	390.4
prasterone formate	413.2	401.8
prasterone propionate	470.2	389.3
prasterone valerate	393.2	391.3
prednisolone	513.0	541.9
prednisone	507.2	527.1
pregnenolone	466.2	445.4
pregnenolone acetate	423.4	425.0
Prodiamine	397.2	407.3
Profluralin	306.2	398.8
progesterone	403.0	429.5
Promecarb	360.2	330.8
Prometon	365.2	380.4
Prometryn	392.2	396.0

propanal	171.3	175.1
propane	85.5	129.4
Propazine	486.2	377.3
propene	88.2	77.5
propionic acid	252.7	256.4
propionitrile	180.4	199.0
Propoxur	360.2	332.9
propranolol	369.2	369.9
propyl 4-aminobenzoate	347.1	336.9
propyl 4-hydroxybenzoate	369.2	339.6
propyl N-phenyl carbamate	331.0	342.3
propylcyclopentane	155.8	222.8
propylene carbonate	218.2	258.5
propylene oxide	161.3	166.5
p-terphenyl	486.3	517.3
p-tolualdehyde oxime	353.2	326.4
p-toluamide	432.2	415.4
p-toluic acid	452.8	452.6
p-toluidine	316.5	312.8
p-tolunitrile	302.2	326.8
p-tolylurea	456.2	443.5
p-xylene	286.3	288.8
pyrazine	328.2	289.3
pyrazole	343.2	334.4
Pyrazosulfuron-ethyl	454.7	453.7
pyrene	423.8	440.1
pyridine	231.5	233.6
pyromellitic dianhydride 1,2,5,6-benzenetetracarboxylic dianhydride	557.2	616.0
pyrrole	249.7	330.7
pyrrolidine	215.3	196.1
quinazoline	320.9	293.4
quinoline	258.4	277.3
quinoxaline	305.7	331.5
Rimsulfuron	450.2	455.4
S-(+)-4-isobutyl-a-methylphenyl acetic acid	325.5	312.9
S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate	322.2	338.2
S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethyl phoshorodithioate	345.3	326.3
S-2,3,3-trichloroallyl diisopropylthiocarbamate	306.4	234.4
S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl-O,O-dimethyl phosphorodithioate	315.1	315.1
sebacic acid	404.0	382.4
Secbumeton	361.2	338.3
sec-butylbenzene	204.2	233.0
secobarbital	373.2	387.7
siduron	409.2	409.2
Simazine	498.2	421.0
Simetryn	356.2	365.5
spiropentane	166.1	182.9
ß,ß-binaphthyl	461.2	492.3
ß-chloroacetic acid	329.2	295.3
ß-chloroacetic acid	329.2	295.3

ß-naphthol	393.6	335.5
ß-naphthyl acetate	342.2	394.1
ß-propiolactone	239.9	220.0
ß-thiolactic acid	291.9	260.7
stanolone acetate	430.0	450.8
stanolone butyrate	364.0	405.7
stanolone formate	415.0	422.7
stanolone propionate	394.2	406.4
stanolone valerate	375.7	405.1
stanozolol	508.2	567.6
styrene	242.3	221.1
suberic acid	415.3	379.8
succinic acid	457.0	370.8
succinimide	400.0	331.2
succinonitrile	331.2	285.4
sulfabenz	473.2	397.7
sulfabenzamide	454.2	473.2
sulfabromomethazine	523.2	523.1
sulfacetamide	456.2	438.9
sulfacytine	440.2	451.2
sulfadiazine	527.2	464.1
sulfadicramide	457.2	454.5
sulfadimethoxine	475.2	475.5
sulfadoxine	465.2	475.5
sulfaethidole	459.2	406.2
sulfalene	449.2	470.4
sulfamerazine	509.2	477.1
sulfameter	488.2	435.5
sulfamethazine	449.2	490.1
sulfamethizole	481.2	445.2
sulfamethomidine	419.2	526.7
sulfamethoxazole	440.2	426.6
sulfamethoxypyridazine	455.2	441.7
sulfamethylthiazole	512.2	464.2
sulfametrole	423.2	471.5
sulfamoxole	467.2	452.5
Sulfanitran	513.2	534.9
Sulfaperine	535.2	477.1
Sulfaphenazole	453.2	492.2
Sulfapyrazine	525.2	464.1
Sulfapyridine	463.2	451.0
Sulfaquinoxaline	520.2	521.9
Sulfasomizole	465.2	465.2
Sulfasymazine	460.2	421.5
Sulfathiazole	475.2	451.2
Sulfazamet	468.2	504.4
Sulfisomidine	516.2	490.1
Sulfisoxazole	467.2	439.6
Sulfometuron-methyl	477.2	449.8
Sulfosulfuron	474.6	492.8
talbutal	382.2	386.7
tebuthiuron	436.2	431.5
teflubenzuron	495.7	467.5

Terbumeton	396.7	410.3
Terbuthylazine	451.2	492.1
Terbutryn	378.2	424.4
terephthalyl dichloride	356.1	351.1
tert-butyl alcohol	299.0	262.2
tert-butyl amine	205.7	244.9
tert-butyl bromide	256.1	272.6
tert-butyl chloride	248.1	252.5
tert-butyl mercaptan	274.4	203.5
tert-butylbenzene	215.0	256.0
tert-butylmethylsulfone	357.6	340.3
testosterone	427.0	420.8
testosterone acetate	413.0	431.4
testosterone butyrate	382.0	390.4
testosterone formate	398.0	401.8
testosterone propionate	393.0	389.3
testosterone valerate	380.0	391.3
testosterone-17-beta-cypionate	374.2	411.0
tetra(methylthia)methane	338.7	244.9
tetrachloroethene	250.8	225.3
tetrachloro-o-xylene	359.2	304.7
tetrachloro-p-xylene	368.2	395.7
tetracontane	353.2	349.7
tetracyanoethylene	472.2	492.7
tetradecane	279.0	280.8
tetradecanoic acid	327.0	333.4
tetrafluoroethylene	142.0	120.7
tetrahydrofuran	164.8	210.6
tetramethylsuccinonitrile	442.0	350.1
tetramethylurea	272.2	227.2
tetramethysuccinic acid	464.0	428.0
tetratriacontane	345.9	342.0
tetrazole	432.1	416.1
theophylline	544.0	579.3
thiacyclobutane	199.9	240.2
thiacyclohexane	292.3	255.6
thiacyclopentane	177.0	248.8
thianthrene	429.6	514.3
Thiazafluron	410.2	372.4
thiazole	239.4	207.0
thidiazuron	486.2	488.2
Thiobencarb	276.5	304.4
Thiofanox	330.2	321.2
thiophene	235.2	215.8
thiophenol	258.2	258.2
thiourea	452.2	452.2
thioxanthene 50-195	401.8	422.6
thioxanthone	487.9	486.6
thymine	321.3	427.7
thymol	324.2	293.9
timolol	475.2	442.4
tolazamide	443.2	443.1
tolbutamide	401.2	366.4

toluene	178.0	233.4
tolyl vinyl sulfone	340.4	321.2
torsemide	436.2	436.9
trans,cis-2,6-octadiene-1,8-dioic acid	380.0	408.6
trans,trans-2,6-octadiene-1,8-dioic acid	541.0	450.4
trans-1-(4-heptanoylphenyl)-4-heptylcyclohexane	344.7	340.9
trans-1,2-cyclohexanediol	372.3	269.8
trans-1,2-dimethylcyclohexane	185.0	175.6
trans-1,3-dimethylcyclohexane	183.1	175.6
trans-1,3-dimethylcyclopentane	139.5	159.7
trans-1,3-pentadiene	185.7	171.5
trans-1,4-dimethylcyclohexane	236.2	175.6
trans-1,4-di-tert-butylcyclohexane	363.2	277.9
trans-10-octadecenoic acid	326.0	319.9
trans-11-octadecenoic acid	317.0	319.9
trans-12-octadecenoic acid	325.0	319.9
trans-13-octadecenoic acid	318.0	319.9
trans-14-octadecenoic acid	327.0	319.9
trans-15-octadecenoic acid	331.0	319.9
trans-1-heptyl-4-(4-nonanoylphenyl)cyclohexane	353.3	346.0
trans-2-butene	167.6	116.2
trans-2-pentene	133.0	100.4
trans-3-octadecenoic acid	334.0	325.4
trans-4-octadecenoic acid	333.0	319.9
trans-5-octadecenoic acid	319.0	319.9
trans-6-octadecenoic acid	326.0	319.9
trans-9-octadecenoic acid (elaidic acid)	317.6	319.9
trans-azobenzene	341.1	410.3
triacontane	338.7	335.4
triamcinolone	543.0	622.0
triamcinolone diacetate	508.0	495.5
triamcinolone hexacetonide	569.2	515.9
triasulfuron	451.3	469.9
triatriacontane	344.0	340.5
tribromomethane	281.5	217.7
trichlormethiazide	543.2	622.3
trichloroacetic acid	330.7	345.1
trichloroethylene	188.5	142.9
trichloromethane	209.6	157.6
tridecandioic acid	387.5	385.3
tridecanoic acid	315.0	329.7
tridecanol	306.6	305.7
Trietazine	374.2	395.6
Triflumuron	468.2	469.7
trifluoroacetonitrile	128.7	195.1
trifluoromethane	118.0	24.2
trifluoromethanethiol	116.0	109.9
trifluoromethyl (2-hydroxy-1-propenyl)ketone	232.4	293.1
Trifluralin	321.7	365.1
trimellitic anhydride(1,2,4-benzenetricarboxylic acid)	438.2	526.5
Trimethacarb	383.2	366.0
trimethylamine	156.1	130.7
trimethylhydrazine	201.2	219.7

trinitroglycerine	285.5	283.3
triphenyl phosphate	322.5	359.0
triphenylamine	400.2	358.3
triphenylchloromethane	376.8	441.7
triphenylene	471.0	572.7
triphenylmethane	365.3	343.1
triphenylphosphine oxide	431.9	431.9
tri-tert-butylmethanol	390.0	497.2
undecanedioic acid	385.0	383.5
undecanoic acid	301.6	331.4
undecanolactone	275.3	300.6
urea	408.1	408.1
vinyl acetate	180.6	137.8
vinyl chloride	119.3	82.2
xanthene	373.7	388.5
xanthone	449.7	452.6
XMC	372.2	353.7
Xylylcarb	352.7	353.7
Z-3-chloro-2-butenoic acid	366.8	347.2
z-enantholactam	310.3	286.0

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