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PARTITION COEFFICIENTS AND THEIR USES

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I. Introduction

A. PURPOSE

In spite of the scientific community's continuing interest over the past 90 years in partitioning measurements, no comprehensive review of the subject has ever been published. In fact, no extensive list of partition coefficients has appeared in the literature. The largest compilation is that of Seidell;[1] smaller compilations have been made by Collander,[2–5] von Metzsch,[6] and Landolt.[7] The task of making a complete listing is nearly impossible since *Chemical Abstracts* has not indexed the majority of the work of the last few decades under the subject of partitioning. While reference may be made under the name of a compound, this is of very little help in organizing a list of known values. Actually, in recent years relatively few partition coefficients have been determined in studies simply devoted to an understanding of the nature of the partition coefficient. The vast majority have been measured for some secondary reason such as the correlation of relative lipophilic character with biological properties of a set of congeners.

In the course of structure–activity studies undertaken by this laboratory over the past decade, many values for partition coefficients of drugs have been found in the biochemical and pharmaceutical literature. From references in these papers, many other values have come to light. As these values have been uncovered, they have been fed into a computer-based "keyed-retrieval" compilation which, while admittedly not complete, is still far more comprehensive than any yet published.

This compilation is not the primary reason for the present review. Work[8] on the correlation of hydrophobic bonding in biochemical systems with partition coefficients has been greatly hindered because of the lack of any survey of the field. This review is written in the hope that the organization of the scattered works on this subject will be of help to others. However, the more dynamic part of the subject is the use of the partition coefficient in the study of intermolecular forces of organic compounds. This subject, while still in the embryonic stage, holds promise for the better understanding of the interaction of small organic molecules with biomacromolecules. Equation 1 is one of many known examples[9] of a

$$\log \frac{1}{C} = 0.75 \log P + 2.30 \qquad \begin{matrix} n & r & s \\ 42 & 0.960 & 0.159 \end{matrix} \qquad (1)$$

linear free energy relationship relating two "partitioning-like" processes. In eq 1, C is the molar concentration of organic compound necessary to produce a 1:1 complex with bovine serum albumin *via* equilibrium dialysis. This partitioning process is related linearly to log P which is the partition coefficient of the compound between octanol and water. The number of molecules studied is represented by n, r is the cor-

(1) A. Seidell, "Solubility of Organic Compounds," Vol. II, 3rd ed, Van Nostrand, Princeton, N. J., 1941.
(2) R. Collander, *Physiol. Plant.*, 7, 420 (1954).
(3) R. Collander, *Acta Chem. Scand.*, 3, 717 (1949).
(4) R. Collander, *ibid.*, 4, 1085 (1950).
(5) R. Collander, *ibid.*, 5, 774 (1951).
(6) F. von Metzsch, *Angew. Chem.*, 65, 586 (1953).
(7) Landolt-Bornstein, "Zahlenwerte and Functionen," Vol. 2, Springer-Verlag, Berlin, 1964, p 698.
(8) C. Hansch, *Accounts Chem. Res.*, 2, 232 (1969).
(9) F. Helmer, K. Kiehs, and C. Hansch, *Biochemistry*, 7, 2858 (1968).

relation coefficient, and s is the standard deviation from regression. Many such linear relationships between solutes partitioned in different solvent systems have been uncovered (section IV). A summary of this work should provide a better understanding of the octanol–water model system and further the application of such linear free energy relationships to "partitioning-like" processes in more complex biological systems.

Another aspect of this review is to summarize the present understanding of the recently discovered[10] additive-constitutive character of the partition coefficient. This property promises to be of value in studying the conformation of molecules in solution.

B. HISTORICAL

The distribution of a solute between two phases in which it is soluble has been an important subject for experimentation and study for many years. In one form or another this technique has been used since earliest times to isolate natural products such as the essences of flowers.

The first systematic study of distribution between two immiscible liquids which led to a theory with predictive capabilities was carried out by Berthelot and Jungfleisch.[11] These investigators accurately measured the amounts present at equilibrium of both I_2 and Br_2 when distributed between CS_2 and water. They also measured the amounts of various organic acids, H_2SO_4, HCl, and NH_3 when distributed between ethyl ether and water. From these early investigations came the first appreciation of the basic fact that the ratio of the *concentrations* of solute distributed between two immiscible solvents was a constant and did not depend on the relative volumes of solutions used.

It was concluded from these early observations that there was a small variation in partition coefficient with temperature, with the more volatile solvent being favored by a temperature decrease. It was also evident that some systems, notably succinic acid partitioned between ether and water, did not obey their simple "rule" even in dilute solution, but they intuitively felt the rule would be justified nonetheless.

In 1891, Nernst made the next significant contribution to the subject.[12] He stressed the fact that the partition coefficient would be constant only if a *single* molecular species were being considered as partitioned between the two phases. Considered in this light, partitioning could be treated by classical thermodynamics as an equilibrium process where the tendency of any single molecular species of solute to leave one solvent and enter another would be a measure of its activity in that solvent and would be related in the usual fashion to the other commonly measured activity functions such as partial pressure, osmotic pressure, and chemical potential. As the primary example of a more exact expression of the "Partition Law," it was shown that benzoic acid distributed itself between benzene and water so that

$$\sqrt{C_s}/C_w = K \qquad (2)$$

where C_s is the concentration of benzoic acid in benzene (chiefly in dimeric form), C_w is the concentration of benzoic acid in water, and K is a constant combining the partition coefficient for the benzoic acid monomer and the dimerization constant for the acid in benzene.[13] Since benzoic acid exists largely as the dimer in benzene at the concentration employed, the monomer concentration in benzene is proportional to the square root of its total concentration in that solvent. Of course, Nernst was also aware that, at low concentrations, the concentration of benzoic acid in the aqueous phase would have to be corrected for ionization.

This association and dissociation of solutes in different phases remains the most vexing problem in studying partition coefficients. For a true partition coefficient, one must consider the same species in each phase. A precise definition of this in the strictest sense is impossible. Since water molecules and solvent molecules will form bonds of varying degrees of firmness with different solutes, any system more complex than rare gases in hydrocarbons and water becomes impossible to define sharply at the molecular level. Very little attention has been given to the fact that solutes other than carboxylic acids may carry one or more water molecules bound to them into the nonaqueous phase. This is quite possible in solvents such as *sec*-butyl alcohol which on a molar basis contains more molecules of water in the butanol phase than butanol!

During the early years of the twentieth century a great number of careful partition experiments were reported in the literature, most of which were carried out with the objective of determining the ionization constant in an aqueous medium of moderately ionized acids and bases. As a point of historical fact, the method did not live up to its early promise, partly because of unexpected association in the organic solvents chosen and partly because of solvent changes which will be discussed in detail in a following section.

After reliable ionization constants became available through other means, partitioning measurements were used to calculate the association constants of organic acids in the nonaqueous phase as a function of the temperature. This yielded values of ΔH, ΔS, and ΔG for the association reaction.[14–18] However, any calculation of self-association constants from partition data alone can be misleading when hydrate formation occurs.[19,20]

As early as 1909, Herz[21] published formulas which related the partition coefficient (P) to the number of extractions necessary to remove a given weight of solute from solution. His formula, with symbols changed to conform to present usage, is as follows.

If W ml of solution contains x_0 g of solute, repeatedly extracted with L ml of a solvent, and x_1 g of solute remains after the first extraction, then $(x_0 - x_1)/L$ = concentration of solute in extracting phase and x_1/W = concentration remaining in original solution.

(10) T. Fujita, J. Iwasa, and C. Hansch, *J. Amer. Chem. Soc.*, **86**, 5175 (1964).
(11) Berthelot and Jungfleisch, *Ann. Chim. Phys.*, 4, 26 (1872).
(12) W. Nernst, *Z. Phys. Chem.*, **8**, 110 (1891).
(13) Occasionally, K values obtained in this fashion have been reported as "partition coefficients." In this report all such values have been corrected to true P values whenever the different terminology was apparent.
(14) M. Davies, P. Jones, D. Patnaik, and E. Moelwyn-Hughes, *J. Chem. Soc.*, 1249 (1951).
(15) J. Banewicz, C. Reed, and M. Levitch, *J. Amer. Chem. Soc.*, **79**, 2693 (1957).
(16) M. Davies and D. Griffiths, *Z. Phys. Chem. (Frankfurt am Main)*, 2, 353 (1954).
(17) M. Davies and D. Griffiths, *J. Chem. Soc.*, 132 (1955).
(18) E. Schrier, M. Pottle, and H. Scheraga, *J. Amer. Chem. Soc.*, **86**, 3444 (1964).
(19) E. N. Lassetre, *Chem. Rev.*, **20**, 259 (1937).
(20) R. Van Duyne, S. Taylor, S. Christian, and H. Affsprung, *J. Phys. Chem.*, **71**, 3427 (1967).
(21) W. Herz, "Der Verteilungssatz," Ferdinand Enke, Stuttgart, 1909, p 5.

$$P = \frac{x_1}{W} \bigg/ \frac{x_0 - x_1}{L}$$

$$x_1 = x_0 \frac{PW}{PW + L}$$

If x_2 is the amount of solute remaining after the second extraction with an equal volume, L, of extractant, then

$$x_2 = x_1 \frac{PW}{PW + L} = x_0 \left[\frac{PW}{PW + L}\right]^2 \tag{3}$$

For the general case where n extractions are made, eq 3 takes the general form

$$x_n = x_0 \left[\frac{PW}{PW + L}\right]^n \tag{4}$$

During the 1940's the mechanical technique of multiple extraction was vastly improved, and countercurrent distribution became an established tool for both the separation and characterization of complex mixtures.[22] It is beyond the scope of this review to deal with the great wealth of literature on this subject. The interested reader may consult the reviews for details.[22,23]

Partition coefficients can be obtained from countercurrent distribution studies and many such values appear in Table XVII. The equation used for such studies is

$$T_{n,r} = \frac{n!}{r!(n - r)!}\left(\frac{1}{P + 1}\right)^n (P)^r \tag{5}$$

where $T_{n,r}$ represents the fraction of the total material in the r tube distributed through n tubes.[24] For distributions involving more than 20 transfers and when P is near unity, the following simpler relationship applies

$$N = n\left(\frac{P}{P + 1}\right) \tag{6}$$

where N = position of peak, n = number of transfers, and P = partition coefficient.

During the two decades bracketing the turn of the century, while the partition coefficient was being studied by physical chemists as an end in itself, pharmacologists became quite interested in the partition coefficient through the work of Meyer[25] and Overton[26] who showed that the relative narcotic activities of drugs often paralleled their oil/water partition coefficients. However, the correlation of so-called nonspecific narcotic activity with partition coefficients did not lead to any really useful generalizations in understanding the mechanism of drug action in the broad sense. Consequently, the interest of both groups in partition coefficients declined greatly. In fact, even the exciting technique of countercurrent distribution did little to stimulate serious studies of partition coefficients *per se*. It is only the recent use of partition coefficients as extrathermodynamic reference parameters for "hydrophobic bonding" in biochemical and pharmacological systems which generated renewed interest in their measurement.[8,9]

(22) L. C. Craig and D. Craig in "Technique of Organic Chemistry," Vol. III, Part I, A. Weissberger, Ed., Interscience, New York, N. Y., 1950, p 171.
(23) L. C. Craig, *Bull. N. Y. Acad. Med.*, **39**, 686 (1963).
(24) B. Williamson and L. Craig, *J. Biol. Chem.*, **168**, 687 (1947).
(25) H. Meyer, *Arch. Exptl. Pathol. Pharmakol.*, 42, 110 (1899).
(26) E. Overton, "Studien uber die Narkose," Fischer, Jena, Germany, 1901.

The symbols and nomenclature associated with partitioning processes have varied considerably. Before the turn of the century, the term "distribution ratio" was often used. Gradually, partition coefficient has become more widely used since *Chemical Abstracts* has indexed under this heading rather than distribution ratio. We shall use partition coefficient when referring to data which have been corrected for ionization, dimerization, etc., so that one is presumably referring to the distribution of a single species between two phases. It is appreciated that there is considerable uncertainty about the nature of "hydrate formation," and attempts to correct partition coefficients for the relative degree of *specific* association with water molecules or solvent molecules are very few. The expression "partition ratio" should be reserved to refer to uncorrected distributions of solute between two phases. Various symbols such as K, K_D, K_P, D, and P have been used to represent the partition coefficient. We have chosen to use P partly because it has become more widely used in recent years than other symbols and because discussions with P very often involve many other equilibrium constants. P stands out from the variety of K values and is more easily followed in discussions, especially since this symbol is used sparingly in the literature pertaining to physical organic chemistry.

II. Theoretical

A. HENRY'S LAW

The most general approach to distribution phenomena is to treat the Partition law as an extension of Henry's law. For a gas in equilibrium with its solution in some solvent

$$m/p = K \tag{7}$$

where m = mass of gas dissolved per unit volume and p = pressure at constant temperature. Since the concentration of molecules in the gaseous phase is proportional to pressure, p can be replaced by C_1 and the mass/unit volume of gas in solution designated by C_2. Equation 7 can then be restated as

$$C_2/C_1 = K \tag{8}$$

In the most general terms, then, the concentrations of *any singular molecular species* in two phases which are in equilibrium with one another will bear a constant ratio to each other as long as the activity coefficients remain relatively constant. The "catch" to the above simple definition is that it assumes no significant solute–solute interactions as well as no strong specific solute–solvent interactions.

Many large interesting organic compounds deviate considerably from ideal behavior in water and various solvents so that one is not always even reasonably sure of the exact nature of the molecular species undergoing partitioning.

B. NONIDEAL BEHAVIOR OF SOLUTES

In many instances solute molecules can exist in different forms in the two phases. This problem can be illustrated with the relatively simple and well-studied case of ammonia.

$$NH_3\text{(vapor)}$$
$$\updownarrow \quad \text{aqueous}$$
$$^1/_2(NH_3)_2 \rightleftharpoons NH_3 \rightleftharpoons NH_4^+\ OH^-$$

In this example, Henry's law is not obeyed, and there is wide variation of m/p (or C_2/C_1) with concentration. Calingaert and

Huggins[27] considered the ionization equilibrium and found that $C_2/[C_1(1 - \alpha)] \cong K$; the degree of ionization is represented by α, and K was found to be constant to within 3% over a 300-fold range of concentrations. Moelwyn-Hughes[28] points out that if one allows for both ionization and dimerization assigning a value of $K = 3.02$ mol/l. for the equilibrium constant for the reaction $2(NH_3) \rightleftarrows (NH_3)_2$, then a constant partition ratio is obtained for concentrations up to 1.6 M.

The equation allowing for both dimerization and ionization can be cast in several forms and the choice is merely one of convenience in handling the data. In treating their data on the distribution of acids between water and toluene, benzene, or chloroform, Smith and White[29] assigned the following symbols in developing a useful set of equations.

C_1 = concentration of total solute in aqueous phase in mol/l.
C_2 = concentration of total solute in organic phase in mol/l. (in terms of monomer molarity)
X = concentration of ions in aqueous phase
N = $C_1 - X_1$ = concentration of un-ionized molecules in water at the first concentration level
n = $C_1' - X_1'$ = concentration of un-ionized molecules in water at the second level
P = concentration single molecules in organic phase/concentration single molecules in aqueous phase
K_D = dissociation constant of double into single molecules in organic phase
K_A = dissociation constant of single molecules into ions in aqueous layer

For aqueous equilibrium

$$K_A = X^2/(C_1 - X)$$

$$\underset{(C_1 - X)}{HA} \rightleftarrows \underset{(X)}{H^+} + \underset{(X)}{A^-}$$

and

$$X = \frac{-K_A + \sqrt{K_A^2 + 4K_AC_1}}{2} \quad (9)$$

For equilibrium in the organic phase[30]

$$(HA)_2 \rightleftarrows 2HA$$

$$K_D = \frac{2(P[C_1 - X_1])^2}{C_2 - P(C_1 - X_1)} = \frac{2(PN)^2}{C_2 - PN} = \frac{2(Pn)^2}{C_2' - Pn} \quad (10)$$

$$P = \frac{C_2n^2 - C_2'N^2}{(n - N)nN} \quad (11)$$

It is readily apparent that any set of experimental values of C_1 and C_2 are apt to have one or more aberrant points, and, furthermore, it is not always apparent how high a concentration must be reached before other solvent effects introduce sizable errors into the relationship which assumes a constancy for the two phases. For this reason it is advisable to recast eq 10 in another form.

$$K_D = 2(PN)^2/(C_2 - PN)$$

which is equivalent to

$$K_D(C_2 - PN) = 2(PN)^2$$

Multiplying by $1/K_DN^2$ and rearranging, we obtain

$$C_2/N^2 = P(1/N) + \text{constant}$$

$$\text{constant} = 2P^2/K_D \quad (12)$$

It is evident that a plot of (C_2/N^2) *vs.* $1/N$ will yield a straight line with slope $= P$. If there are sufficient data points, any aberrant values will be apparent, and the concentration beyond which the linear relationship no longer holds is more obvious.

A good deal of the data on acids in the literature had never been treated in this manner. To make these calculations from data which recorded a range of *total* concentrations in each phase (regardless of whether present as dimer, ion, etc.), we have written a small computer program to calculate $1/N$ and C_2/N^2 for each concentration value and P for each consecutive set of two concentrations. The program also punches a set of cards with C_2/N^2 and $1/N$ values which can then be used with a regression program to eliminate aberrant values and values beyond the true linear relationship. Whenever possible, the P values in Table XVII have been calculated in this way and 95% confidence intervals have been placed on them. P values so obtained were used to calculate K_D values in Table II.

A slightly altered form of eq 12 has also been widely used.[14,31] Stated in terms of the above symbols, it is

$$\frac{C_2}{N} = P + \frac{2P^2}{K_D}N \quad (13)$$

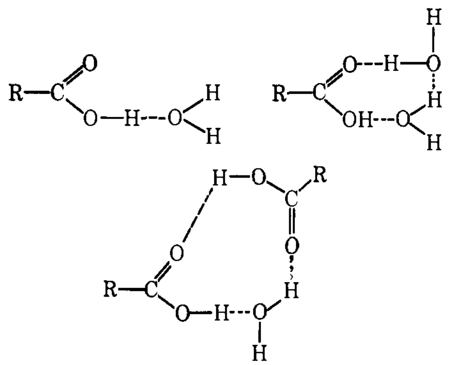
In this form a plot of N *vs.* $1/N$ yields the value of P from the intercept (the partition coefficient at zero concentration where dimerization can be ignored). The value of the dimer dissociation constant can be obtained from P and the slope. It is obvious that dividing both sides of eq 13 by N yields an equation of the form of eq 12 and thus a given set of data should yield the same values for P and K_D by either method of calculation. We prefer to use the Smith and White equations, especially where no data points were measured at low concentrations and where, therefore, there can be a wider 95% confidence interval in the intercept value as compared to the confidence interval on the slope.

In calculating partition coefficients or association constants of acids, one is of course quite dependent on the quality of equilibrium constants available. For example, Moelwyn-Hughes,[32] in reviewing data reported by Rothmund and Drucker,[33] assumed no dimerization of picric acid in benzene and obtained a value of 0.143 for the ionization constant of picric acid in water. If, on the other hand, we accept the value of 0.222 for the K_A of picric acid as determined by conductivity measurements[34] and recalculate Rothmund and Drucker's data, a P value of 48.77 is found instead of 31.78. The K_D value, as calculated by eq 12, is very nearly infinity; *i.e.*, there is very little association in the benzene phase. This is a departure from the behavior of unsubstituted phenols in benzene. Endo[35] used partitioning data to show that the dissociation constant for the phenol trimer in benzene is approximately 1.

Ionization and self-association are not the only fates which can befall the carboxylic acid monomer (or other polar molecules) and complicate the calculation of the true partition coefficient and association constant.[19,20] If the solute forms a

(27) G. Calingaert and F. Huggins, Jr., *J. Amer. Chem. Soc.*, **45**, 915 (1923).
(28) E. A. Moelwyn-Hughes, "Physical Chemistry," 2nd ed, Pergamon Press, New York, N. Y., 1961, p 1085.
(29) H. Smith and T. White, *J. Phys. Chem.*, **33**, 1953 (1929).
(30) In eq 10, Smith and White omitted 2 in the numerator.
(31) Reference 28, p 1081.
(32) Reference 28, p 1082.
(33) V. Rothmund and K. Drucker, *Z. Phys. Chem.*, **46**, 827 (1903).
(34) J. Dippy, S. Hughes, and L. Laxton, *J. Chem. Soc.*, 2995 (1956).
(35) K. Endo, *Bull. Chem. Soc. Jap.*, **1**, 25 (1926).

firmly bonded hydrate, there is another set of equilibria to worry about in the organic phase. In order to best explain variation of P with concentration in the system of benzoic acid distributed between benzene and water, it was proposed[20] that three hydrates are present in the benzene. By a rather complex



curve-fitting technique using solubility data of water in benzene and benzoic acid in benzene, equilibrium constants for the three types of hydrates were estimated. In Table I the association constants and partition coefficients for benzoic acid in benzene are given, and the results assuming hydrate formation are compared with results neglecting it. It is evident from Table I that the calculations which take hydrate formation into account affect the partition coefficient as well as the dimerization constant. However, if method B[20] is accepted, it does not yield values far out of line from those determined by other investigators.

Table I

Hydration and Dimerization of Benzoic Acid in Benzene

	Temp, C°	K_D	*P*
Van Duyne, *et al.*[20]			
Method A	25	589	0.95
Method B	25	298	1.31
Schilow and Lepin[36]	23.5	109	2.30
Smith[37]	25	260[a]	1.63
Huq and Lodhi[38]	25	244	1.56
Hendrixson[39]	10	?	1.43
Hendrixson[39]	40	?	2.10

[a] An average of six different determinations.

Although preferred by Van Duyne, *et al.*, method A is open to criticism for it assumes that the dimerization constant (K_{20} in their paper) is the same in dry benzene as in "wet." Completely apart from any tendency to encourage hydrate formation, the addition of water to benzene could be expected to increase the dielectric constant and by this means alone should lower K_D (association).[19,40] However, it must be admitted that there is evidence which supports a lesser or negligible role for a change from a "dry" to a wet organic solvent.[14]

In Table II are listed a number of association constants for carboxylic acids in various solvents calculated according to the method discussed above. Sometimes K_{assoc} was found to vary with concentration at levels below 5×10^{-3} M, and in these cases the constant value at higher concentrations was chosen. The variation at the lower concentrations may be more a function of the analytical techniques employed in measurement rather than a meaningful physical phenomenon, although this is by no means completely clear from the data. One must keep the arguments of Van Duyne, *et al.*,[20] in mind when considering these constants. If hydrate formation is always involved with carboxylic acids in solvents such as benzene, then the association constants of Table II will generally be too low.

Not much in the way of useful generalizations can be made from the data in Table II. It is of interest that there is a general trend of the degree of dimerization by solvents: toluene > benzene > chloroform ≫ ether. The fact that benzene values are lower than toluene is likely due to the greater solubility of water in benzene. In fact, the solubility of water in the organic solvent as seen from Table VIII is in inverse order to the degree of dimerization, water being most soluble in ether and least soluble in toluene.

Considering a single solvent, toluene, the dimerization constant appears to increase with the size of the alkyl group, at least up through valeric acid. This effect seems to correlate most closely with Taft's steric parameter, E_s. While eq 14 is

$$\log P_{assoc} = -0.470(\pm 0.32)E_s + 1.989(\pm 0.20) \qquad (14)$$

n	*r*	*s*
8	0.824	0.223

quite significant statistically ($F_{1,6} = 12.6$), the correlation is not very high. It does suggest, however, that the steric effect of the alkyl moiety of the acid is most important. Adding a term in pK_a to eq 14 does not improve the correlation. One cannot place a great deal of confidence in eq 14 since there is considerable overlap between the two parameters, pK_a and E_s, for the set of acids under consideration ($r^2 = 0.834$). Equation 14 does suggest that the large alkyl groups might inhibit hydrate formation and in this way favor dimerization.

There is little trend to be seen in the scattered group of halo fatty acids and substituted benzoic acids, but the statement[40] that the more highly chlorinated acids are more highly associated does *not* seem supported.

In the development of eq 12 and 13 it was assumed that association in the organic phase proceeded no further than the dimer stage. For the case of acetic acid in the benzene–water system, it has been shown[16] that neither partition coefficient nor the dimerization constant values calculated from this type of expression would be markedly altered if some trimer or tetramer were also formed. These authors calculated K_{1-3} to be 2.35×10^{-4}, but suggest that this might well be viewed as a correction in the dimerization equilibrium constant and therefore not have any real molecular significance.

While there is little or no evidence for association beyond the dimer state for low molecular weight carboxylic acids, other types of solutes have a greater associative tendency. For instance, a sudden increase in P^{*}[50] (apparent partition coeffi-

(36) N. Schilow and L. Lepin, *Z. Phys. Chem.*, **101**, 353 (1922).
(37) H. W. Smith, *J. Phys. Chem.*, 26, 256 (1922).
(38) A. K. M. S. Huq and S. A. K. Lodhi, *ibid.*, **70**, 1354 (1966).
(39) W. S. Hendrixson, *Z. Anorg. Chem.*, **13**, 73 (1897).
(40) C. Brown and A. Mathieson, *J. Phys. Chem.*, **58**, 1057 (1954).
(41) N. A. Kolossowsky and I. Megenine, *Bull. Soc. Chim. Fr.*, **51**, 1000 (1932).
(42) W. Herz and H. Fischer, *Chem. Ber.*, **38**, 1138 (1905).
(43) N. A. Kolossowsky and S. F. Kulikov, *Z. Phys. Chem.*, **A169**, 459 (1934).
(44) F. S. Brown and C. R. Bury, *J. Chem. Soc.*, **123**, 2430 (1923).

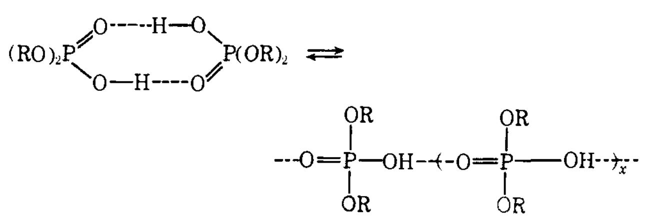
Table II

Association Constants of Acids

Acid	Toluene K_{assoc}	Toluene Ref	Benzene K_{assoc}	Benzene Ref	$CHCl_3$ K_{assoc}	$CHCl_3$ Ref	K_{assoc}	Other solvent	Ref
1. Formic	29	41	121^a	45	26	45	0.6	Nitrobenzene	48
				45					
2. Acetic	42	42	28	42	60	45	43	CCl_4	45
							0	Ether	46
3. Propionic	133	29	94	29	31	29	78	Xylene	46
							0.5	Ether	49
4. Butyric	182	29	97	29	52	29	2^a	Xylene	46
5. Isobutyric	300	29	182	29	64	29			
6. Valeric	200	29	140	29	49	29			
7. Isovaleric	225	29	138	29	80	29			
8. Hexanoic	94	29	96	29	30	29	160	Xylene	46
							0.1	Ether	49
9. Isohexanoic			68	29	50	29			
10. Crotonic	450	29	271	29	136	29	419	Xylene	46
11. Chloroacetic	132^a	43			96^a	43	1.6	Nitrobenzene	43
	4.5	42	2.2	42					
12. Bromoacetic	0	29	0	29	53	46			
13. Iodoacetic	60	29	37	29	16	29			
14. β-Chloropropionic	100	29	55	29	35	29			
15. α-Bromopropionic	30	29	16	29	9.5	29			
16. β-Bromopropionic	65	29	61	29	25	29			
17. β-Iodopropionic	133	29	95	29	64	29			
18. α-Bromobutyric	47	29	22	29	22	29			
19. Dichloroacetic	44	43					157	CCl_4	43
							0	Ether	43
20. Trichloroacetic	0	43			0	43	0	Ether	46
							0	Nitrobenzene	43
21. Picric	0	36	0.6	33	0	47			
		42							
22. Benzoic	79	29	295	37	33	29	0	Ether	46
			298	20	120	17	1440	Xylene	46
			108	36					
23. *o*-Toluic	21	29			1	29			
24. *p*-Toluic	291	29			3.3	29			
25. *o*-Methoxybenzoic	3.9	29			0	29			
26. *p*-Methoxybenzoic	82	29			0.3	29			
27. *o*-Chlorobenzoic	106	29			11	29	312	Xylene	46
28. *m*-Chlorobenzoic	25	29			0	29			
29. *p*-Chlorobenzoic	0	29			0	29			
30. *o*-Nitrobenzoic	0	29			1	29			
31. *m*-Nitrobenzoic	78	29			61	29	133	Xylene	46
32. *p*-Nitrobenzoic	0	29			0	29			
33. *o*-Bromobenzoic					30	29			
34. *m*-Bromobenzoic					0	29			
35. Salicylic	17	29			44	29	57	Xylene	46
36. Acetylsalicylic	143	29			75	29			
37. Methylanthranilic					85	29			
38. Phenylacetic	145	29	151	29	56	29			
39. Anthranilic					770	29			

^{a} Doubtful value.

cient or partition ratio) of dibutyl phosphate in hexane (when $C_{org} = 0.05\ M$) can be explained in terms of the conversion of the dimer to a polymer chain.



For solutes showing negligible ionization (the work with the phosphate esters was done in 0.1 M HNO_3) in the aqueous phase, it is easy to test if a higher polymer is formed in the organic phase. It has been pointed out[35] that if a trimer is formed

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(46) H. W. Smith, *J. Phys. Chem.*, **25**, 204, 605 (1921).
(47) W. Herz and M. Lewy, *Z. Elektrochem.*, **46**, 818 (1905).
(48) N. A. Kolossowsky and A. Bekturov, *Bull. Soc. Chim. Fr.*, **2**, 460 (1935).
(49) W. U. Behrens, *Z. Anal. Chem.*, **69**, 97 (1926).
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$$K_{assoc} = C_{tr}/(C_{mon})^3 \qquad (15)$$

where C_{tr} = concentration trimer in organic phase and C_{mon} = concentration monomer in organic phase. Hence

$$C_{app} = C_{mon} + 3C_{tr} = C_{mon} + 3K_{assoc}C_{mon}^3 \qquad (16)$$

where C_{app} = total concentration solute in organic phase (regardless of form), and C_w = concentration in water phase (no polymerization). Assuming trimer cannot exist in the aqueous phase, the true partition coefficient for monomer is

$$P = C_{mon}/C_w$$

Therefore

$$C_{app} = PC_w + 3K_{assoc}(PC_w)^3$$

$$P^* = P + 3K_{assoc}P^3C_w^2 \qquad (17)$$

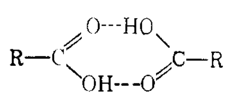
A plot of the apparent partition coefficient, P^*, *vs.* the water concentration squared, C_w^2, should give a straight line with the intercept yielding the value P and the slope yielding the value K_{assoc}.

Many investigators have followed similar derivations, but some have not limited the applications to relatively un-ionized solutes. For example, Almquist[51] observed a straight line plot of C_o/C_w *vs.* C_w with picric acid in the chloroform–water system. Assuming the applicability of the general relationship

$$C_o/C_w = n(K_{assoc}P^nC^{n-1}) + P \qquad (18)$$

he calculated that the true partition coefficient was 0.46 and the association constant was 8.6. However, if we use the measured ionization constant for picric acid, we get constant values of P = 15.8 and K_{assoc} = 0. As pointed out above, picric acid is apparently not associated in benzene, and we would expect it to be even less associated in chloroform. Furthermore, the value of 15 for P fits in much better when compared to the octanol–water system by means of the regression equation A in Table VIII.

Most investigators have assumed that the amount of dimerization of aliphatic acids in the aqueous phase is insignificant, an assumption which seems reasonable if only a head-to-head dimer is possible.



However, with higher homologs other possibilities exist. Micelle formation becomes quite significant even at low concentrations with long-chain fatty acids.[52] Even though one works at concentrations below the critical micelle concentration (cmc), the problem of association in the aqueous phase cannot be eliminated. Entwinement of the long alkyl chains occurs in very dilute solutions.[53] Careful examination of cryoscopic data, Raman spectra, and vapor pressure measurements[16,54,55] have been interpreted to yield aqueous phase dimerization constants for carboxylic acids which increase with chain length: formic, 0.04; acetic, 0.16; propionic, 0.23; butyric, 0.36. From a careful study of the distribution of acetic acid in the benzene–water system, it was concluded[16] that the dimer association constant in water is only one-fifth this large (*i.e.*, 0.033). Nevertheless, the effect becomes quite large with dodecanoic acid, making the determination of a true monomer partition coefficient almost impossible.[56] Thus the present data have not completely eliminated the possibility of head-to-head dimerization of fatty acids in the aqueous phase, but the preponderance of new evidence[18] favors the "chain entwinement" viewpoint.

Distribution studies have also been made with other types of solutes which are known to form micelles at relatively low concentrations in water such as alkylpyridinium and pyridonium chlorides and *p-tert*-octylphenoxypolyoxyethanol surfactants. Over a range of solute concentrations *below cmc*, constant P values have been observed.[57,58]

C. THERMODYNAMICS OF PARTITIONING SYSTEMS

Solvent systems which are almost completely immiscible (*e.g.*, alkanes–water) are fairly well behaved and lend themselves to more rigorous thermodynamic treatment of partitioning data than solvent systems which are partially soluble in each other.[17,59,60] The following development can be applied more strictly to the former systems, but the departures from ideality exhibited by the more polar solvent systems are not so great as to render this approach valueless. They will be discussed later. It should be noted here that the *thermodynamic* partition coefficient is a ratio of mole fractions ($P' = X_o/X_w$), and it should not be confused with the more common expression of P which is a dimensionless ratio of concentrations.

Cratin[61] has presented a lucid discussion of some of the aspects of the thermodynamics of the partitioning process. The following discussion is drawn from his analysis which relies heavily on extrathermodynamic assumptions.

For each of the "i" components comprising an ideal solution, the following equation is assumed to hold

$$\mu_i(T,P,X) = \mu_i^\theta(T,P) + RT \ln X_i \qquad (19)$$

where μ_i^θ is the chemical potential of pure "i" in the solution under specified conditions, and X_i is its mole fraction. μ_i^θ is not the actual chemical potential of pure "i" but the value it would have if the solution remained ideal up to X_i = 1. It can be shown[61] that, for dilute solutions, the chemical potential based on mole fractions is larger than that based on molar concentrations by a factor of $RT \ln \bar{V}_s°$, where $V_s°$ is the molar volume of solvent and therefore

$$\mu_i(T,P,X) = \mu_i^\theta(T,P) + RT \ln \bar{V}_s° + RT \ln C_i \qquad (20)$$

An interesting approach to the study of the intermolecular forces involved in partitioning is to assume that the free energy of transfer of a molecule can be factored into the contributions of its various parts; that is, P is an additive-constitutive property of a molecule (see section V). Cratin[61] considered the thermodynamic implications of this concept. Assuming that the total transfer free energy of a molecule (μ_t) is made up of a

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(52) J. L. Kavanau, "Structure and Function in Biological Membranes," Vol. I, Holden-Day, San Francisco, Calif., 1965, p 11.
(53) P. Mukerjee, K. J. Mysels, and C. I. Dulin, *J. Phys. Chem.*, 62, 1390 (1958).
(54) A. Katchalsky, H. Eisenberg, and S. Lifson, *J. Amer. Chem. Soc.*, 73, 5889 (1951).
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(56) C. Church and C. Hansch, unpublished results.
(57) E. Crook, D. Fordyce, and G. Trebbi, *J. Colloid Sci.*, 20, 191 (1965).
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(59) R. Aveyard and R. Mitchell, *Trans. Faraday Soc.*, 65, 2645 (1969).
(60) R. Aveyard and R. Mitchell, *ibid.*, 66, 37 (1970).
(61) P. D. Cratin, *Ind. Eng. Chem.*, 60, 14 (1968).

lipophilic component (μ_L) and n hydrophilic groups (μ_H), we may write

$$\mu_t(w) = \mu_L(w) + n\mu_H(w)$$

$$\mu_t(o) = \mu_L(o) + n\mu_H(o)$$

Assuming ideal behavior

$$\mu_t(w) = \mu_L{}^{\theta}(w) + n\mu_H{}^{\theta}(w) + RT \ln X(w)$$

$$\mu_t(o) = \mu_L{}^{\theta}(o) + n\mu_H{}^{\theta}(o) + RT \ln X(o)$$

Converting from mole fractions to concentration terms, the above equations become

$$\mu_t(w) = \mu_L{}^{\theta}(w) + n\mu_H{}^{\theta}(w) + RT \ln \bar{V}^\circ(w) + RT \ln C(w)$$

$$\mu_t(o) = \mu_L{}^{\theta}(o) + n\mu_H{}^{\theta}(o) + RT \ln \bar{V}^\circ(o) + RT \ln C(o)$$

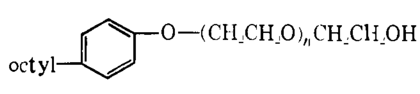
At equilibrium $\mu_t(w) = \mu_t(o)$; hence equating equations, collecting terms, and replacing $C(o)/C(w)$ by P, we obtain

$$[\mu_L{}^{\theta}(w) - \mu_L{}^{\theta}(o)] + RT \ln [\bar{V}^\circ(w)/\bar{V}^\circ(o)] + n[\mu_H{}^{\theta}(w) - \mu_H{}^{\theta}(o)] = +RT \ln P \quad (21)$$

Setting $\Delta\mu^{\theta} = \mu^{\theta}(w) - \mu^{\theta}(o)$, eq 21 takes the form

$$\log P = \frac{n\Delta\mu_H{}^{\theta}}{2.3RT} + \frac{\Delta\mu_L{}^{\theta}}{2.3RT} + \log [\bar{V}^\circ(w)/\bar{V}^\circ(o)] \quad (22)$$

If eq 22 holds, a plot of log P *vs.* n will be linear with a slope equal to $\Delta\mu_H{}^{\theta}/2.3RT$ and an intercept of $\Delta\mu_L{}^{\theta}/2.3RT$ + log $[\bar{V}^\circ(w)/\bar{V}^\circ(o)]$. Cratin illustrated the validity of eq 22 by plotting the data of Crook, Fordyce, and Trebbi[57] for *tert*-octylphenoxyethoxyethanols of the type



partitioned between isooctane and water. Compounds with n varying from 1 to 10 were studied. A good linear relation was obtained from $n = 3$ to $n = 10$. A slight departure from linearity for $n = 1$ and 2 was found. The linear relationship between n and P is given as[58]

$$\log P = -0.442n + 3.836 \quad (23)$$

From eq 23 the standard free energy change (25°) for the transfer of a mole of $-CH_2CH_2O-$ from isooctane to water is -0.602 kcal and the free energy change (o → w) for the *p-tert*-octylphenoxyethoxy group is +6.52 kcal/mol. Of course since the partitioning data on the phenoxyethoxyethanols were obtained at a single constant temperature, this is not a very rigorous test of eq 22 since under this condition, $\bar{V}^\circ(o)/\bar{V}^\circ(w)$ will also be constant. Nevertheless, eq 22 does define the necessary conditions for additivity of log P values. The standard free energy of transfer of solute in the partitioning process is given by

$$\Delta G_{tr}{}^{\theta} = \Delta\bar{\mu}^{\theta} = RT \ln P' \quad (24)$$

With the usual assumption that the standard molar enthalpy change is not temperature dependent in the range studied,[61] it is true that

$$\frac{\partial \ln P'}{T} = \frac{\Delta\bar{H}^{\theta}}{RT^2} \quad (25)$$

where $\Delta\bar{H}^{\theta}$ is equivalent to the standard enthalpy of transfer between the two solvents. It is thus possible to calculate this enthalpy of transfer by measuring P' over a range of temperatures. In practice this is rather imprecise because of two implied assumptions: first, that the levels of each solvent dissolved in the other remain constant over the temperature range; second, if P is measured in terms of concentrations, that the ratio of solvent molar volumes remains constant also. For this reason the preferred method of obtaining the enthalpy of transfer is by measuring the heats of solution in two separate solvents, whence

$$\Delta\bar{\mu}^\circ = \Delta\bar{H}_{tr}{}^\circ = \Delta H^\circ(w) - \Delta H^\circ(o) \quad (26)$$

The entropy of transfer can, of course, be calculated from

$$\Delta G_{tr}{}^\circ = \Delta H_{tr}{}^\circ - T\Delta S_{tr}{}^\circ \quad (27)$$

Aveyard and Mitchell[59,60] have performed these calculations for aliphatic acids and alcohols partitioned between alkanes and water. They find much greater enthalpies for the alcohols which they ascribe to the "dehydration" of the OH function during transfer. Although the acids are also "dehydrated," they are thought to recover much of this energy in the hydrogen bonding of dimerization. The corresponding ΔS values for the acids are much smaller than for the alcohols, and thus the net free energy changes are not greatly different.

The changes in miscibility of more polar solvent systems as a function of solute concentration have been studied in only a few systems.[62-64] However, experience has shown that the partition coefficient at low solute concentrations is usually not highly dependent on this effect. Even with solvent pairs as miscible as isobutyl alcohol-water, the effect is small with solutes at 0.01 *M* or less, and solvent pairs less miscible than chloroform-water will easily tolerate 0.1 *M* solute without appreciable miscibility changes.

Equation 25 shows how one would expect the partition coefficient to vary with temperature. However, it is not very enlightening from a practical point of view, for the necessary heats of solution are rarely available and, furthermore, there is the added unknown of the dependence of solvent molar volume on temperature. The effect of temperature on P is not great if the solvents are not very miscible with each other. A summary in Table III of results of varying degrees of accuracy for a variety of solutes in different solvent systems indicates the effect is usually of the order of 0.01 log unit/deg and may be either positive or negative. Insufficient data are present to attempt any useful generalizations.

D. ENERGY REQUIREMENTS FOR PHASE TRANSFER

The relative roles of the various binding forces which determine the way a solute distributes itself between two phases

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Table III

Temperature Effect on Log *P*

Solvent–water	*Solute*[a]	*Temp, °C*	*Δ log P/deg*	*Ref*
Octanol	Hexanoic acid	4-22	1.7×10^{-3}	56
	Octanoic acid	4–22	0.0	56
	n-Butylpyridinium bromide	4–22	-1.0×10^{-2}	65
	n-Tetradecylpyridinium bromide	4–22	-1.0×10^{-2}	65
Ethyl ether	Acetic acid	0–25	-1.2×10^{-3}	66
	Succinic acid	15–25	-0.9×10^{-2}	62
Chloroform	Acetyl-*d*-leucine	4–27	-0.9×10^{-2}	67
	Acetyl-*d*-leucine	24–37	-1.3×10^{-2}	67
	Methylamine	18–32	1.0×10^{-2}	68
	Ammonia	18–32	0.8×10^{-2}	68
Oil				
Olive	Antipyrine	7–36.5	1.2×10^{-2}	69
Cod-liver	Antipyrine	7–36.5	1.5×10^{-2}	69
Cottonseed	Ethanol	3–30	1.1×10^{-2}	70
Benzene	*o*-Phenylenediamine	20–70	3.4×10^{-3}	71
	p-Phenylenediamine	20–70	4.4×10^{-3}	71
	p-Nitrosomethylaniline	6–25	2.1×10^{-3}	72
	Acetic acid	6–18.5	3.0×10^{-3}	66
Xylene	2-Methyl-5-ethylpyridine	10-30	4.5×10^{-3}	73
	2-Methyl-5-ethylpyridine	30–50	7.0×10^{-3}	73
Toluene	2-Methyl-5-ethylpyridine	10–30	7.5×10^{-3}	73
	2-Methyl-5-ethylpyridine	30–50	-4.0×10^{-3}	73
	Ethylamine	18–32	1.7×10^{-2}	68
	Diethylamine	18–32	1.9×10^{-2}	68
	Triethylamine	18–32	1.9×10^{-2}	68
1-Hexanol	Malonic acid	20–60	-1.2×10^{-3}	74
	Succinic acid	20–60	-0.5×10^{-3}	74
Heptane	*p*-Chloroaniline	15–35	5.5×10^{-3}	75
Isooctane	*p-tert*-Octylphenoxynonaethoxyethanol (OPE-9)	25–60	2.8×10^{-2}	58
		Average =	9.0×10^{-3}	

[a] No correction made for $\Delta pK_a/dT$ for any of the acids.

has been examined by a number of authors.[76] Kauzmann[77] has given a particularly clear summary of this thinking, especially from the point of view of the interaction of small molecules with proteins, and the following discussion relies heavily on his summary.

The study of the hydrocarbons in water shows that although the ΔH of solution is negative (indicating a favorable enthalpy change by the evolution of heat), such compounds are notoriously insoluble in water. This reluctance to mix with water is a result of a large ΔS for the process. It is this large energy of reordering the hydrocarbon solute and the water solvent molecules which keeps them in separate phases when placed together. The same phenomenon regulates the distribution of apolar solute molecules in an apolar solvent–water system. Table IV[77] illustrates this point.

Table IV

Thermodynamic Changes in Hydrocarbon Transfer

	T	ΔS_u[a]	ΔH	ΔG_u[a]
CH_4 in benzene → CH_4 in H_2O	298	−18	−2800	+2600
CH_4 in ether → CH_4 in H_2O	298	−19	−2400	+3300
CH_4 in CCl_4 → CH_4 in H_2O	298	−18	−2500	+2900
Liquid propane → C_3H_8 in H_2O	298	−23	−1800	+5050
Liquid butane → C_4H_{10} in H_2O	298	−23	−1000	+5850
Liquid benzene → C_6H_6 in H_2O	291	−14	0	+4070
Liquid toluene → C_7H_8 in H_2O	291	−16	0	+4650
Liquid ethybenzene → C_8H_{10} in H_2O	291	−19	0	+5500

[a] S_u and G_u refer to the unitary entropy and free energy in cal/mol.

A variety of work, less well defined than that of Table IV, supports the conclusion that the entropic component of ΔG plays a large role in the position of equilibrium (partition coefficient) taken by nonpolar compounds in nonpolar water–solvent systems. Kauzmann has put forward the following facts.

1. Mixtures of lower aliphatic alcohols with water show positive deviations from Raoult's law, indicating an increase in unitary free energy ($\Delta G_\mu > 0$) for the transfer of alcohol from alcohol to water phase, this despite the fact that heat is evolved ($\Delta H < 0$) on the addition of these alcohols to water. Therefore $\Delta S_u = (\Delta H_u - \Delta G_u)/T < 0$ when an alcohol molecule is transferred to water.

2. The solubilities of many liquid aliphatic compounds (*e.g.*, 3-pentanone, butanol, ethyl acetate, ethyl bromide) in water decrease with increase in temperature. Hence ΔH for the transfer process must, according to the principle of Le Chatelier, be <0. The fact that some of these substances are extremely soluble in water means that $\Delta G_u > 0$. Therefore, ΔS_u for the mixing must be negative. Similar to this is the

(75) A. Aboul-Seoud and A. El-Hady, *Rec. Trav. Chim. Pays-Bas*, **81**, 958 (1962).
(76) H. Frank and M. Evans, *J. Chem. Phys.*, **13**, 507 (1945).
(77) W. Kauzmann, *Advan. Protein Chem.*, **14**, 37 (1959).

fact that on heating aqueous solutions of such compounds as nicotine, *sec*-butyl alcohol, etc., separation into two phases results at temperatures not far above room temperature.

3. The formation of micelles from detergent molecules in water is accompanied by very small heat changes; that is to say, the dissociation of micelles into individual molecules does not depend on a large positive value of ΔH. Hence it is assumed that this association–dissociation reaction is controlled largely by a large negative ΔS.

The origin of the large negative unitary entropy change and the small negative enthalpy change involved in partitioning between aqueous and nonaqueous phases was first clearly appreciated by Frank and Evans. They reached the conclusion that when organic compounds are placed in water, the water molecules arrange themselves around the apolar parts in what was termed "iceberg" structures. The word "iceberg" was, perhaps, not too well chosen for it was not meant to imply that the structure was as rigid or as extensive as in pure ice, and it differed further in being denser rather than lighter than water. This is apparent from the data in Table V.[77]

Table V

Volume Changes in Transfering Hydrocarbons from Nonpolar Solvents to Water

	ΔV, *ml/mol*
CH_4 in hexane → CH_4 in H_2O	−22.7
C_2H_6 in hexane → C_2H_6 in H_2O	−18.1
Liquid propane → C_3H_8 in H_2O	−21.0
Liquid benzene → C_6H_6 in H_2O	−6.2

These structures were later referred to as "flickering clusters" to indicate their lack of stability. Since the entropy lost in freezing a mole of water is 5.3 cal/deg and the unitary entropy loss per mole of hydrocarbon entering the aqueous phase is only 20 cal/deg (see Table IV), either only four or five molecules are associated with each hydrocarbon unit or the structure is less firm than in pure ice.

The Frank–Evans point of view is that the stripping of the form-fitting sweater[78] of water molecules from the apolar part of the solute results in a large entropy change in the randomization of the water molecules. An alternative point of view is that of Aranow and Witten.[79] They reason that in the aqueous phase the apolar chain of a solute molecule is rigidly held in a favored rotational configuration by the structured layer of water molecules surrounding it. In the organic solvent its rotational oscillations are relatively unrestricted. They write the canonical single particle partition function, Z, for a molecule having n carbon-to-carbon bonds in the *apolar* environment as

$$Zn = \psi\left(\sum_i e^{-\epsilon_i/kT}\right)^n \qquad (28)$$

Because of the threefold increase in the number of energy levels, the corresponding partition function in the water phase is

$$Zn = \psi\left(\sum_i 3e^{-\langle\epsilon_i\rangle/kT}\right)^n \qquad (29)$$

The partition coefficient per $-CH_2-$ in an alkyl chain can then be defined as

$$P = \frac{\psi_\alpha}{\psi_\beta}\frac{\left(\sum_j 3e^{-\langle\epsilon_i\rangle/kT}\right)^n}{\left(\sum_i e^{-\epsilon_i/kT}\right)^n} \qquad (30)$$

where α and β refer to the organic and aqueous phases, respectively. This is assuming that the motions of internal rotation are separable from all other motions and that the internal rotation contribution has been assumed representable as the product of n equivalent factors. At room temperature, if kT is much smaller than the spacing between $\langle\epsilon_0\rangle$ and $\langle\epsilon_1\rangle$ or between ϵ_0 and ϵ_1, then $P \cong (\psi_\alpha/\psi_\beta)3n(e^{-\langle\epsilon_0\rangle-\epsilon_0/kT})^n$. If ψ_α/ψ_β varies little with n and $\langle\epsilon_0\rangle \sim \epsilon_0$

$$P_n/P_{n-1} \cong 3 \text{ or } \log P_{(CH_2)} \cong 0.5$$

Aranow and Witten present partition data to show that the difference in P values between adjacent members in a homologous set of fatty acids is about 3. This factor has also been observed by others[4,9,80] for a variety of homologous series.

A $-CF_2-$ group would be expected to affect its environment a great deal more than a $-CH_2-$ unit would,[79] but it still has a very similar geometry. Therefore, it was predicted that the P values of a hydrocarbon chain should differ from a fluorocarbon chain if the flickering cluster theory holds, but should be nearly the same if Aranow and Witten's theory holds. The following set (Table VI) of partition coefficients

Table VI

Octanol–Water Partition Coefficients of Fluoro Compounds[a]

	Log P	Δ *log P/CF₂*
1. CF_3CH_2OH	0.41 ± 0.03	
		0.82
2. $CF_3CF_2CH_2OH$	1.23 ± 0.06	
		0.58
3. $CF_3CF_2CF_2CH_2OH$	1.81 ± 0.06	
4. $CF_3COOC_2H_5$	1.18 ± 0.04	
		0.94
5. $CF_3CF_2COOC_2H_5$	2.12 ± 0.04	

[a] Log P values are the result of four separate determinations made at room temperature using vapor-phase chromatography for analysis. Unpublished data: C. Church, F. Helmer, and C. Hansch.

throws some light on the problem.

In comparing compounds 1 and 2, for example, one must keep in mind the fact that the electron-withdrawing groups, when placed near elements containing lone pair electrons, usually raise the partition coefficient by an increment greater than simple additivity.[10] However, σ_I for CF_3 is 0.41 and σ_I for C_2F_5 is 0.41[81] so that this effect is ruled out. Two of the three values are considerably higher than the value of $0.5/CF_2$ predicted by the Aranow–Witten hypothesis. and therefore the partitioning data favor the Frank–Evans hypothesis.

Hydrogen bonding is the next factor to consider in studying the energy requirements for phase transfer. This factor is of paramount importance in determining the character of both the solute and the organic solvent phase. Compounds such as

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(80) C. Hansch and S. M. Anderson, *J. Org. Chem.*, **32**, 2583 (1967).
(81) W. A. Sheppard, *J. Amer. Chem. Soc.*, **87**, 2410 (1965).

alcohols, esters, and ketones have quite different properties than hydrocarbons. Moreover, as solvents, it is not simply the hydrogen bonding character of the pure compound which must be considered. One must keep in mind that rather large amounts of water (especially when figured in molar terms) are present in these oxygen-containing solvents when saturated during the partititoning process (see Table VIII). For example, octanol dissolves in water only to the extent of 0.0045 *M*. However, the molar concentration of water in octanol is 2.30. The transfer of an alcohol or acid from the water phase to a hydrocarbon phase may involve complete "dehydration" of the polar OH or COOH function, It seems highly unlikely that such complete "dehydration" would occur in, say, butanol which is 9 *M* with respect to water content at saturation. Even in octanol, which is 2.3 *M* with respect to water at saturation, it is likely that most highly polar functions would be more or less solvated by water and/or the hydroxyl function of the alcohol.

Certain solvents such as alcohols and amines can act as both donors and acceptors in hydrogen bonding. This increases their versatility as solvents. For this reason Meyer and Hemmi[82] suggested using oleyl alcohol–water partition coefficients as a reference system for evaluating partitioning of drugs in biological systems. Earlier workers had used esters (olive oil, cotton seed oil, etc.) to represent lipophilic biophases. Since many NH and OH groups are present in enzymes and membranes, it is not surprising that alcohol–water systems give better correlations and thus have become more widely used as extrathermodynamic reference systems.

Other intermolecular forces which must be considered in the partitioning process are dispersion forces arising out of electron correlation. It seems that these would play a minor role in setting equilibrium positions of solutes. Dispersion forces involved in complex formation in solution will largely cancel out since, when a solute molecule leaves one phase and enters a new phase, it exchanges one set of London interactions for another.[83]

The energy required to transfer from the aqueous phase to the organic phase any solute which contains two or more formal charges is obviously going to depend heavily on the dielectric constant of the particular organic phase in question. Most of the water-immiscible organic solvents have dielectric constants much lower than that of water, and thus charged solutes must contain rather large hydrocarbon residues to have positive log *P* values. This combination makes them very surface active and usually results in difficulties of measurement.

Amphoteric molecules such as amino acids, tetracycline, or the sulfa drugs are most lipophilic when they contain an equal number of positive and negative charges. Typical dependence of log *P* upon pH is shown in Figure 1.

For bases which can accept one or more hydrogen ions, A^{n+}, the partition coefficient, $P_{A^{n+}}$, is related to the partition coefficient of an associated strong acid, P_{H^+}, by the expression

$$P_{A^{n+}} = k[P_{H^+}]^n \quad (31)$$

This relationship for the 2-butanol–water system has been verified[84] by measuring $P_{A^{n+}}$ of ammonia, alanine, L-arginine, and L-histidyl-L-histidine, as well as P_{H^+} of the strong acids $HOEtSO_3H$, CH_3SO_3H, HCl, HBr, HNO_3, and $HClO_4$. A log–log plot of the *P* values gave a series of straight lines with a slope of 1 for ammonia and alanine, 2 for L-arginine, and 3 for L-histidyl-L-histidine.

(82) K. H. Meyer and H. Hemmi, *Biochem. Z.*, 277, 39 (1935).
(83) R. S. Mulliken and W. B. Person, *J. Amer. Chem. Soc.*, **91**, 3409 (1969).
(84) F. Carpenter, W. McGregor, and J. Close, *ibid.*, **81**, 849 (1959).

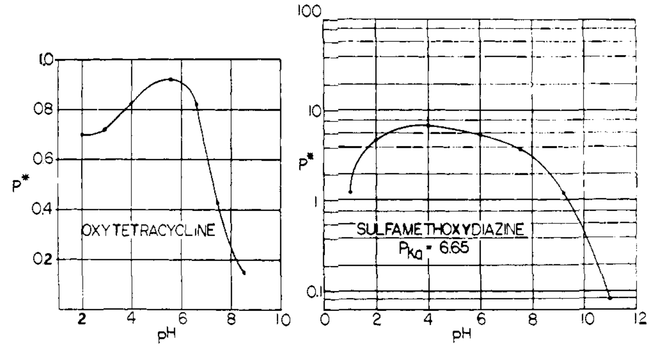

Figure 1. Variation of apparent partition coefficient with pH: (left) J. Colaizzi and P. Klink, *J. Pharm. Sci.*, **58**, 1184 (1969); (right) W. Scholtan, *Arzneim.-Forsch.*, **18**, 505 (1968).

Solutes which are ionized and completely dissociated in the aqueous phase present additional complications to the treatment of partitioning as strictly an equilbrium process, such as given in section II. The identity of the solute species in both phases is rarely assured. If electrical conductivity resulted solely from the current-carrying capability of single ions, then salts in organic solvents with relatively high dielectric constants (*e.g.*, nitrobenzene, 36.1; or nitromethane, 39.4) could be considered to be over 90% dissociated into single ions at 10^{-3} *M*.[85,86] But as the dielectric constant decreases, the mutual energy of configurations where there are three ions in contact ($A^-C^+A^-$) becomes comparable to kT.[87] At this point they are thermally stable and capable of carrying current, and therefore conductance is not proof *per se* of complete dissociation.

Even relatively hydrophilic ion pairs can be accommodated in a lipophilic solvent such as cyclohexane if this solvent contains a small amount of a dipolar solvating agent. In the instance where the cation is the large lipophilic member of the pair, the most effective solvating agents appear to be those with acidic protons, *e.g.*, chloroform, alcohols, and phenols.[88] In the reverse situation where the small cationic charge is unshielded, solvating species with nucleophilic sites (*e.g.*, ethers, ketones, amides, and phosphate esters) are most effective.

In considering the partitioning of carboxylic acids and amines, it is convenient to work with the Δ log *P* resulting from the addition or removal of a proton to create an ion. (This is analogous to the definition of π values taken up on p 542.) By this convention, $\Delta \log P = (\log P_{ion}) - (\log P_{neutral})$ and will always have a negative sign for the more polar ion is obviously more hydrophilic.

For aliphatic acids, Δ log *P* is about −4.06; for salicylic, it is −3.09; for *p*-phenylbenzoic, it is −4.04. For a simple aliphatic amine (dodecyl), the Δ log *P* of protonation is −3.28.

(85) H. Falkenhagen, "Electrolyte," S. Herzel, Leipzig, 1932.
(86) J. C. Philip and H. B. Oakley, *J. Chem. Soc.*, **125**, 1189 (1924).
(87) R. Fuoss and F. Accascina, "Electrolytic Conductance," Interscience, New York, N. Y., 1959, p 222.
(88) T. Higuchi, A. Michaelis, T. Tan, and A. Hurwitz, *Anal. Chem.*, **39**, 974 (1967).

For amines containing an aromatic ring, the Δ log P_{H^+} values tend to vary (see Table XVII):

phenothiazines = −3.65
$C_6H_5(CH_2)_3NH_2$ = −2.92
procaine = −4.14

Protonating an aromatic nitrogen appears intermediate; *e.g.*, for acridine, Δ log P_{H^+} = −3.90. Very little difference in the octanol–water log *P* was observed for the amine salts whether the anion was chloride, bromide, or iodide.

It should be noted that if one wishes to measure the log $P_{octanol}$ of a dissociable organic ion, he must buffer the system more than 4 pH units away from the pK_a in most cases. The actual ratio of ionic to neutral form in the organic phase can be determined from the following expressions:

$$\log \frac{[A^-]}{[HA]}(\text{org}) = (\log P_{ion} - \log P_{neutral}) - (pK_a - pH)$$

$$\log \frac{[BH^+]}{[B]}(\text{org}) = (\log P_{ion} - \log P_{neutral}) - (pH - pK_a)$$

For example, in partitioning an aliphatic carboxylic acid with a pK_a of 4.5 and the aqueous phase buffered at pH 8.5, only $^1/_{10,000}$th of the acid will be in the neutral form in the aqueous phase, and yet almost one-half of that present in the octanol phase will be the un-ionized species.

Since the difference in log *P* between the ionic and neutral forms of solutes partitioned in other solvent systems is likely to be *greater* than that noted for octanol–water, it is even more difficult to directly measure the *P* values for ions in these systems. For instance, in partitioning codeine between $CHCl_3$ and an aqueous phase 0.1 and 1.0 *N* in HCl, the assumption was made that in neither case was the measured value distorted by any free amine in the organic phase.[89] However, values from Table XVII indicate that the log P_{CHCl_3} of the free amine would be about 5.0 units higher than the hydrochloride, and therefore a pK_a − pH difference of 5 units (pK_a = 6.04; pH = 1) is *not* sufficient to assure that only ion pairs are being partitioned.

It is somewhat unexpected to find the log *P* for the $\geqslant N^+$–CH_3 group lower than that of the $\geqslant N^+$–H group. In this case, the nature of the anion appears to make a small but real difference in the log $P_{octanol}$ value. (For *N*-hexadecylpyridinium, Δ log P_{Br-Cl} = 0.12.) The following Δ log $P_{octanol}$ values were observed for adding both a methyl group and a positive charge to an amine:

	Δ *log P*	*Anion*
Chlorpromazine	−5.35	Cl^-
Pyridine	−5.00	Br^-
$C_6H_5(CH_2)_3N(CH_3)_2$	−4.75	I^-

The partition coefficient of ions between a nonpolar solvent and water plays an essential role in the application of these solvents as liquid ion-exchange membranes for ion-selective electrodes.[90] A lipophilic anion, such as oleate, dissolved in the solvent nitrobenzene can serve as the "site" species; see Figure 2. In theory, the selectivity among various cations is completely independent of the chemical properties of the "site" species and depends solely on the difference in partition coefficient of the ions in that solvent.[90] For instance, the partition coefficient of monovalent cations between any alcohol and water are not greatly different,[91] and therefore these solvents are not useful in liquid membrane electrodes. The partition coefficients in nitrobenzene, however, are markedly different,[92] and this solvent has been employed in a useful electrode to measure [Li^+] in the presence of [Rb^+].[90] The partition coefficients for the iodides fall in the following order: $Li^+ < Na^+ < K^+ < Rb^+ < Et_4N^+ < Bu_4N^+$, which is the order also found for the solvent system diisopropyl ketone–water.[93]

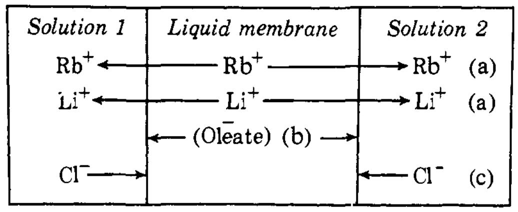

Figure 2. Ion-selective electrode (oleate in nitrobenzene): (a) Counterions which differ in log *P;* (b) the site ion (for an anion-selective electrode, dodecyl amine might be chosen); (c) co-ion.

Using dodecylamine as a site species, the order of anion sensitivity in a nitrobenzene membrane sytem is $I^- > Br^- > Cl^- > F^-$.[90] This is the same order as the partition coefficients of the anions measured in that solvent.[92]

For ideal behavior in a liquid membrane electrode, the site ion should be almost completely "trapped" within the organic phase, resulting in almost negligible exchange of co-ion; see Figure 2. Ideal behavior is also dependent upon complete dissociation of the site ions in the organic phase, and the concentration of site ions at which departure from ideality is noted may be a useful measure of the onset of association into ion pairs. Ion selectivity depends only slightly upon ion mobility and rates of diffusion across phase boundaries.[94]

Like nitrobenzene–water, the chloroform–water system gives a wide range of *P* values for the counterions associated with any large organic ion.[95–97] This again raises the question of which system should one choose for a hydrophobic parameter to be used in correlating biological activity. Perhaps if one is investigating electrical potentials in isolated nerve tissue, for example, an ion-selective system might give values which rationalize more of the data. Yet it is widely accepted[98] that with most drugs the biological response in the intact animal is only slightly dependent upon the nature of the counterion (as long as initial solubility is achieved), and thus a model system which is not ion selective should be preferred.

The distinction between ion-selective partitioning systems and the nonselective systems may be simply that the former have aprotic organic phases. In an extensive study of ion solvation in protic *vs.* aprotic solvents, it has been shown[99]

(89) G. Schill, R. Modin, and B. A. Persson, *Acta Pharm. Suecica,* **2,** 119 (1965).
(90) G. Eisenman in "Ion Selective Electrodes," No. 314, R. Durst, Ed., National Bureau of Standards, Washington, D. C., 1969, pp 4–8.
(91) H. Ting, G. Bertrand, and D. Sears, *Biophys. J.,* **6,** 813 (1966).
(92) J. T. Davies, *J. Phys. Chem.,* **54,** 185 (1950).
(93) F. Karpfen and J. Randles, *Trans. Faraday Soc.,* **49,** 823 (1953).
(94) H. L. Rosano, P. Duby, and J. H. Schulman, *J. Phys. Chem.,* **65,** 1704 (1961).
(95) R. Bock and G. Beilstein, *Z. Anal. Chem.,* **192,** 44 (1963).
(96) R. Bock and C. Hummel, *ibid.,* **198,** 176 (1963).
(97) R. Bock and J. Jainz, *ibid.,* **198,** 315 (1963).
(98) A. Albert, "Selective Toxicity," 2nd ed, Wiley, New York, N. Y., 1960, p 116.
(99) A. J. Parker, *Quart. Rev. Chem. Soc.,* 163 (1962).

that anion solvation by protic solvents decrease strongly in the order $F^- > Cl^- > Br^- > I^- >$ picrate$^-$, while in aprotic solvents the order is reversed. Even though for this study methanol was used as the standard protic solvent (rather than water) and a ratio of solubilities rather than a partition coefficient measured solvent affinity, these data are quite relevant to this review. They predict the large range and correct order of P values for the above anions in the nitrobenzene–water system and predict a very small range in any alcohol–water system (nonprotic *vs.* protic solvents). The solvation values for cations[100] would predict a smaller protic *vs.* aprotic difference, but the methanol *vs.* dimethylformamide values place them in the expected order: $Na^+ < K^+ < Cs^+ < Et_4N^+ < Bu_4N^+$.

III. Experimental Methods

By far the most extensive and useful partition coefficient data were obtained by simply shaking a solute with two immiscible solvents and then analyzing the solute concentration in one or both phases. However, mention should be made of some other fundamentally different techniques.

Occasionally the ratio of solubilities in two separate solvents has been measured and reported as a partition coefficient.[101] This is truly a value of P only at saturation and is apt to be quite different from the value obtained under the conditions of low solute concentration and with the two phases mutually saturated. As seen from Table VIII, the amount of water soluble in many solvents can be quite high and this modifies their solvent character considerably. Rather high concentrations of organic solutes are necessary to saturate many solvents. Not only does this make for greater solute–solute interactions, but such high concentrations actually change the character of the organic phase so that one is no longer dealing with, say, butanol as the organic phase but with some mixed solvent. However, if the information desired relates to miscible solvents,[99,100] then there is little choice in the matter. An extensive study has been made of the solubility ratios of amino acids in a series of alcohols, and this should be consulted for experimental details.[102,103]

Another procedure[104] of limited application is that of placing a volatile solute such as ethanol in a closed system with two other solvents which need not be immiscible. If the concentration of solute is determined in both solutions and if the relation between solute activity and concentration is known in one of the solutions, the dependence of activity on concentration in the other can be inferred. This method, which resembles solvent isopiestic procedures, can be used at low solute concentrations.

A rapid method which employs automatic titration for the determination of partition coefficients of organic bases between immiscible solvents has been described.[105] To an aqueous solution of the base hydrochloride, sufficient standard NaOH is added to convert about 20% to the free base. The automatic titrator is then operated as a pH-Stat, and, when the immiscible solvent is added and stirred, it removes only free base from the aqueous phase. From the ratio of NaOH added prior to the addition of organic solvent, the partition ratio can be calculated.

Some solutes with surfactant properties cause troublesome emulsions to form between two immiscible solvents. Usually these can be dispersed by centrifugation or long standing or a combination of both. If this fails, diffusion techniques can be used, although they are distressingly time consuming. This method[58] has yielded results consistent with other procedures. It has also been shown[57] how a partition coefficient can be calculated from the difference between surface and interfacial tensions, but the accuracy is probably not better than an order of magnitude.

It has been mentioned that Craig countercurrent distribution procedures often yield valuable partition coefficient data. However, for purposes of characterizing or separating a particular substance, it is desirable[106] to work with a partition coefficient near 1. This is often accomplished through the use of mixed solvents. Also, when a clean separation of solute compounds is desired, concentrated buffers are used[106] to give maximum shift of P with pH. As a result, many of the partition coefficients calculated from Craig procedures have little comparative value because the solvent is unique or because the aqueous phase is at high ionic strength.

A perusal of the literature reveals that many different techniques have been employed for the simple problem of mixing and separating the two phases in order to obtain an equilibrium distribution of the solute. Many workers have used periods of shaking as long as an hour or more. Such a lengthy procedure is unnecessary. It has been found[107] that simple repeated inversion of a tube with the two phases establishes equilibrium in 1–2 min. With almost all of the many substances studied by these authors, equilibrium was reached with 50 inversions. Experience in our laboratory has shown that about 100 inversions in roughly 5 min produce consistent results. Very vigorous shaking should be avoided since this tends to produce troublesome emulsions. The clarity of the two phases is not a dependable criterion of the absence of an emulsion, and therefore a centrifugation step is recommended for precise determinations. This cannot be overemphasized. For convenience, partitioning can be carried out in 250-ml centrifuge bottles fitted with glass stoppers. In this way centrifugation can be accomplished without transfer of material. Avoiding cork or rubber stoppers eliminates the possibility that impurities might be introduced by these materials or that some substances might be extracted by such stoppers. Since it is desirable to work at low concentrations in each phase (0.01 M or less), small amounts of impurities can cause serious error.

In measuring about 800 partition coefficients between water and octanol we have usually analyzed the solute in only one phase and obtained the concentration in the other by difference. However, if there is the possibility that absorption to glass may occur, both phases must be analyzed. Such absorption has been found to occur with ionic solutes.[108] Ab-

(100) R. Alexander, E. C. F. Ko, A. J. Parker, and T. J. Broxton, *J. Amer. Chem. Soc.*, **90**, 5049 (1968).
(101) B. Wroth and E. Reid, *ibid.*, **38**, 2316 (1916).
(102) E. Cohn and J. Edsal, "Proteins, Amino Acids and Peptides," Reinhold, New York, N. Y., 1943, p 200.
(103) T. McMeekin, E. Cohn, and J. Weare, *J. Amer. Chem. Soc.*, **58**, 2173 (1936).
(104) S. D. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, *J. Chem. Educ.*, 40, 419 (1963).
(105) A. Brandstrom, *Acta Chem. Scand.*, 17, 1218 (1963).
(106) L. Craig, G. Hogeboom, F. Carpenter, and V. DuVigneaud, *J. Biol. Chem.*, **168**, 665 (1947).
(107) Reference 22, p 159.
(108) J. Fogh, P. O. H. Rasmussen, and K. Skadhauge, *Anal. Chem.*, **26**, 392 (1954).

sorption may also be a serious problem when working with very low concentrations of labeled compounds ($<10^{-6}$ *M*).

It is quite helpful to estimate the partition coefficient in advance of the determination (see section V). This allows one to make a more judicious estimate of the volumes of solvents to employ. With very lipophilic molecules, for example, it is evident that relatively small volumes of nonpolar solvent must be used or there will be insufficient material left in the aqueous phase for analysis. For example, if a solute is thought to have a *P* value of 200, and 20 mg was partitioned between equal 100-ml volumes, the aqueous phase would end up with only 0.1 mg. If the analytical procedure has an inherent error of 0.05 mg/100 ml, the *P* value could vary between 133 and 400. If, however, 200 ml of water and 5 ml of nonpolar solvent were used, the water layer would contain 3.5 mg or 1.75 mg/100 ml and the same analytical accuracy would limit the range of *P* values from 194 to 206. With good analytical procedures and proper volume choices of solvent, log *P* values in the range -5 to $+5$ can be measured.

As pointed out in section II.C, many partitioning systems show temperature dependence of about 0.01 log unit/deg in the room-temperature range. Obviously, temperature control is essential for highest accuracy and is most important for the more miscible systems. For most applications, especially as an extrathermodynamic parameter for biological structure–activity relationships, variations due to temperature are hardly comparable to those inherent in the other measurements, and therefore we do not consider it a serious shortcoming that most of the values in Table XVII are simply "at room temperature" without an estimation of what that might be.

IV. Linear Free-Energy Relationships among Systems

Since partition coefficients are equilibrium constants, it should not be surprising that one finds extrathermodynamic[109] relationships between values in different solvent systems. Such an assumption was implicit in the work of Meyer[25] and Overton[26] who used oil–water partition coefficients to correlate the narcotic action of drugs. Smith[46] also showed the possibility of such relationships, but Collander[5] was the first to express the relationship in precise terms.

$$\log P_2 = a \log P_1 + b \qquad (32)$$

Working with only his own partitioning data, Collander examined only the linear relationship between similar solvent systems. In particular, he showed that eq 32 held between the systems isobutyl alcohol–water, isopentyl alcohol–water, octanol–water, and oleyl alcohol–water. Hansch,[110] using Smith's data, later extended the comparison of relatively nonpolar systems using $CHCl_3$–water for P_1 and the following systems for P_2: CCl_4, xylene, benzene, and isoamyl acetate.

The most useful relationships for the study of solute–solvent interactions are obtained by defining a reference system and making it the independent variable, P_1, in a set of equations of the form of eq 32. Most of the reasons behind our choice of octanol–water as the reference system have already been given, but another practical one is the fact that it is the system with the largest number of measured values containing the widest selection of functional groups. Furthermore, a large portion of these measurements have been made in one laboratory, and therefore should be more self-consistent.

It is clearly evident from Smith's data[46] that, when the nonpolar phases of the partitioning systems differ widely, and especially when the solute sets contain molecules which cannot hydrogen bond along with those which can, eq 32 does *not* give a good correlation. For example, in comparing benzene–water with octanol–water, 52 assorted solutes give a regression equation with a poor correlation coefficient (0.81) and high standard deviation (0.55).

It might seem feasible to place all solutes in the order of a ratio of *P* values from two standard systems and group them, if possible, on this basis. This can be useful when the objective, for example, is limited to a comparison of Lewis acid strengths by using the ratio of *P* values between a saturated and unsaturated solvent system, hexane *vs.* *p*-xylene.[111] Sandell[112] used a similar ratio from the $CHCl_3$ and diethyl ether systems to reach some general conclusions about the relative percentage of tautomeric forms of various solutes, but this simplified system failed when applied to certain specific cases. For example, it erroneously predicted a sizable concentration of imino form in a solution of benzenesulfonamide.[113] Infrared spectroscopy data[114,115] appear to directly contradict this conclusion.

It appeared that the simplest way to make such a separation of solute types was to take the values from a single equation and separate all the "minus deviants" into one category and the "plus deviants" into another. After one has done this for several solvent systems, one finds that the strong hydrogen bond donors are the "minus deviants" and the hydrogen bond acceptors are the "plus deviants." The ether–water system is exceptional, for while it also segregates the donors from acceptors, the deviations are reversed.

Some work has been done to establish a scale of values for H donors[116] and H acceptors,[117] but these cover only a small fraction of the solutes appearing in Table XVII. A reasonable alternative was to place some of the more common functional groups into "general solute classes" which would be compatible with the "plus deviant" and "minus deviant" catagories as indicated by regression analysis. These classes also had to be compatible with the well-known rules based on the electronegativity and size of the two atoms bound by the hydrogen atom;[118] see Table VII.

It is to be expected that some changes in molecular structure *outside of the functional group* will have important effects on H bonding, sufficient at times to change the assigned solute class. Examples of this situation which have been allowed for are seen in no. 5 and 13, but others can be expected also.

Whenever a solute molecule contained two or more noninteracting functional groups, each of which would require classification as "A" and "B", we have placed it in the class

(109) J. E. Leffler and E. Grunwald, "Rates and Equilibria of Organic Reactions," Wiley, New York, N. Y., 1963.
(110) C. Hansch, *Farmaco, Ed. Sci.*, 23, 294 (1968).
(111) R. Orye, R. Weimer, and J. Prausnitz, *Science*, **148**, 74 (1965).
(112) K. Sandell, *Naturwissenschaften*, **53**, 330 (1966).
(113) K. Sandell, *Monatsh. Chem.*, **92**, 1066 (1961).
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(117) R. W. Taft, D. Gurka, L. Joris, P. von R. Schleyer, and J. W. Rakshys, *J. Amer. Chem. Soc.*, 91, 4794, 4801 (1969).
(118) G. Pimentel and A. McClellan, "The Hydrogen Bond," Reinhold, New York, N. Y., 1960, p 229.

Table VII

General Solute Classes

Group "A" H donors		1. Acids
		2. Phenols
	c	3. Barbiturates
	c	4. Alcohols
	c	5. Amides (negatively substituted, but not di-N-substituted)
	c	6. Sulfonamides
	c	7. Nitriles
	c	8. Imides
	c	9.[a] Amides
Group "B" H acceptors		10.[a] Aromatic amines (not di-N-substituted)
		11. Miscellaneous acceptors
		12. Aromatic hydrocarbons
		13. Intramolecular H bonds[b]
		14. Ethers
		15. Esters
		16. Ketones
		17. Aliphatic amines and imines
		18. Tertiary amines (including ring N compounds)

[a] Classes 9 and 10 must be reversed when considering the ether and oil solvent systems. [b] *E.g.*, *o*-nitrophenol. [c] "Neutral" in $CHCl_3$ and CCl_4.

which gave the best fit with that particular equation. It was felt that the best fit of the data would serve to categorize the dominant solvation forces in such cases. For example, *p*-methoxybenzoic acid is both an acid (class 1) and an ether (class 14). Regression equation "A" gave the best fit in the solvent systems: benzene, toluene, and xylene (see Table VIII). This suggests that the H-donor ability of the carboxyl group dominates in placing *p*-methoxybenzoic acid in the most poorly accommodated category when these solvents are compared to octanol. In the $CHCl_3$-water system, however, *p*-methoxybenzoic acid is not so poorly accommodated (again in relation to the standard reference system), and actually the "N" equation fits it as well as the "A" (Table VIII). This suggests that the weak H-donor capability of the solvent, $CHCl_3$, increases the accommodation of this solute by interacting with the ethereal oxygen.

Once a practical basis for sorting solutes was available, we could study the set of equations (of the form of eq 32) relating the solvent systems to see if the slope and intercept values could give some indication of the solute–solvent forces at work. In doing so, it was convenient to establish some sort of preliminary order to the solvent systems. Although the dipole moment, the dielectric constant, the solubility parameter,[119–122] and the molar attraction constant have each been useful in establishing a scale for solvents in certain applications, none seemed to put partitioning solvent systems into a sensible order. A simple scheme which did work was to order them according to the amount of water they contained at saturation. In Table VIII they appear in this order.

In using the slopes and intercepts of the equations of Table VIII to study solute–solvent interactions as compared to the standard solute–octanol interaction, we can consider the *slope* value first. We can see that it is a measure of the solvent system's sensitivity to changes in lipophilicity of solutes. Butanol—water, as expected, has the lowest slope value and the least sensitivity. When this pair is saturated with one another, they are about as much alike as two separate phases can be. Since log *P* measures the difference in transfer energy between the two, changes in solute character will register as only small differences when compared to octanol.

Increasing the hydrocarbon chain length in the solvent alcohol increases the dissimilarity of the alcohol–water phases, and there is an increased sensitivity to solute changes. Apparently, a maximum sensitivity is reached at octanol for the slope in the oleyl alcohol equation is also 1.0.

There is some basis for the postulate that the partitioning process, outside of hydrogen bonding, is the same for solutes in each system, and therefore if hydrogen bonding were accounted for separately, the slopes of all the equations in Table VIII would be near 1.0. Some of the results reported by Higuchi and his coworkers[116] can be interpreted in this manner. They have used the cyclohexane–water system where the organic phase has a minimum of hydrogen-bonding ability, and to it have added a small amount of tributyl phosphate (TBP) or isopropoxymethyl phosphoryl fluoride (sarin) as H-bond acceptors. By partitioning a set of substituted phenols between the two phases they have calculated an equilibrium constant for the solute–TBP complex. Table IX contains their data and log $P_{octanol}$ values for the phenols, and from it eq 33 and 34 have been formulated. The correlation be-

$$\log P_{octanol} = 0.50 \log P_{cyclobexane} + 2.43 \qquad (33)$$

n	*r*	*s*
9	0.791	0.391

$$\log P_{octanol} = 1.00 \log P_{cyclohexane} + 1.20 \log K_{HB} + 2.35 \quad (34)$$

n	*r*	*s*
9	0.979	0.140

tween partition coefficients in octanol and cyclohexane is poor, as shown by eq 33. However, when correction is made for the hydrogen-bonding ability of the phenols by adding a term in log K_{HB}, a good correlation is obtained (eq 34). Moreover, the coefficient with log $P_{cyclobexane}$ is 1.00, indicating that in a rough sense the desolvation processes are the same for each system.

It is reasonable to propose that decreasing the lipophilic character of the nonaqueous phase decreases the energy required to transfer a hydrocarbon solute (or a specific segment of a solute, such as a methylene group) from the nonaqueous to the aqueous phase, and this would result in a decrease in the slope values in Table VIII in going from octanol to butanol. It would be logical to predict, therefore, that any alteration of the aqueous phase in these partitioning systems to make it more like the nonaqueous would also reduce the transfer energy and lower the slope.

There are not a great deal of data in the literature which are suitable for testing this hypothesis, but the investigations of Feltkamp[125] certainly support it. He measured the distribution of various barbiturates between diethyl ether and a 50:50 mixture of dimethylformamide and water. Since DMF itself is not very well accommodated by ether (log $P_{ether-water}$

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(122) J. A. Ostrenga, *ibid.*, 58, 1281 (1969).

(123) *P* values for all of the solutes used to develop the equations are listed in *J. Org. Chem.*, 36, 1539 (1971), microfilm edition.
(124) D. Burton, K. Clark, and G. Gray, *J. Chem. Soc.*, 1315 (1964).
(125) H. Feltkamp, *Arzneim.-Forsch.*, 15, 238 (1965).

Table VIII

Solvent Regression Equations[123]

$\text{Log } P_{solv} = a \text{ Log } P_{octanol} + b$

Solvent (vs. H_2O)	H_2O concn at saturation, 10^3M	H-donor solutes, Equation "A": a[a]	b[a]	n	r	s	H-acceptor solutes, Equation "B": a	b	n	r	s
Cyclohexane	2.5	0.675 (±0.24)	− 1.842 (±0.48)	26	0.761	0.503	1.063 (±0.12)	− 0.734 (±0.25)	30	0.957	0.360
Heptane	3.3	1.056 (±0.73)	− 2.851 (±1.46)	10	0.764	0.916	1.848 (±0.44)	− 2.223 (±0.93)	11	0.954	0.534
CCl_4[b]	10.0	1.168 (±0.12)	− 2.163 (±0.15)	24	0.974	0.282	1.207 (±0.27)	− 0.219 (±0.37)	11	0.959	0.347
Xylene	18.8	0.942 (±0.13)	− 1.694 (±0.21)	19	0.963	0.225	1.027 (±0.08)	− 0.595 (±0.16)	21	0.986	0.230
Toluene	25.6	1.135 (±0.11)	− 1.777 (±0.16)	22	0.980	0.194	1.398 (±0.22)	− 0.922 (±0.37)	14	0.971	0.274
Benzene	26.0	1.015 (±0.11)	− 1.402 (±0.14)	33	0.962	0.234	1.223 (±0.19)	− 0.573 (±0.20)	19	0.958	0.291
$CHCl_3$[c]	68.4	1.126 (±0.12)	− 1.343 (±0.21)	28	0.967	0.308	1.276 (±0.14)	+ 0.171 (±0.17)	21	0.976	0.251
Oils[d]	72.5	1.099 (±0.06)	− 1.310 (±0.09)	65	0.981	0.271	1.119 (±0.11)	− 0.325 (±0.19)	14	0.988	0.233
Nitrobenzene	180	1.176 (±0.23)	− 1.072 (±0.20)	9	0.977	0.217					
Isopentyl acetate	456	1.027 (±0.08)	+ 0.072 (±0.13)	22	0.986	0.209					
Ether	690	1.130 (±0.04)	− 0.170 (±0.05)	71	0.988	0.186	1.142 (±0.13)	− 1.070 (±0.12)	32	0.957	0.326
				"Sole" Equation							
Oleyl alcohol	712	0.999 (±0.06)	− 0.575 (±0.11)	37	0.985	0.225					
Methyl isobutyl ketone	950	1.094 (±0.07)	+ 0.050 (±0.11)	17	0.993	0.184					
Ethyl acetate	1620	0.932 (±0.21)	+ 0.052 (±0.18)	9	0.969	0.202					
Octanol	2300	1.000	+ 0.000								
Cyclohexanone	4490	1.035 (±0.20)	+ 0.896 (±0.30)	10	0.972	0.340					
Primary pentanols	5000[e]	0.808 (±0.07)	+ 0.271 (±0.09)	19	0.987	0.161					
sec- and *tert-*pentanols	5320[f]	0.892 (±0.06)	+ 0.288 (±0.06)	11	0.996	0.091					
2-Butanone	5460	0.493 (±0.07)	+ 0.315 (±0.07)	9	0.987	0.093					
Cyclohexanol	6510	0.745 (±0.09)	+ 0.866 (±0.14)	12	0.985	0.100					
Primary butanols	9440[g]	0.697 (±0.02)	+ 0.381 (±0.03)	57	0.993	0.123					

[a] The values in parentheses are the 95% confidence intervals. [b] The "N" equation is $\log P_{CCl_4} = 0.862\ (\pm 0.60) \log P_{octanol} - 0.626\ (\pm 0.70)$ ($n = 6$, $r = 0.809$, $s = 0.462$). [c] The "N" equation is $\log P_{CHCl_3} = 1.10\ (\pm 0.09) \log P_{octanol} - 0.617\ (\pm 0.12)$ ($n = 32$, $r = 0.974$, $s = 0.254$). [d] Most liquid glyceryl triesters fit this equation; olive, cottonseed, and peanut oils were the most frequently used. [e] *n*-Amyl alcohol = 5.03 *M* in water; isoamyl alcohol = 4.50 *M* in water. [f] Water content measured for 2-pentanol only. [g] Water content measured for 1-butanol only.

= −1.62),[2] it should not greatly change the solvent properties of the water-saturated ether phase, but it must greatly reduce the protic nature of the aqueous phase. The following equation was derived using this rather limited set of solutes.

$$\log P_{ether/H_2O-DMF} = -0.321 + 0.400 \log P_{octanol}$$

n	r	s
6	0.988	0.058

The equation with two additional values for hexobarbital and phenobarbital was essentially the same (slope = 0.405) even though these poorly predicted solutes lowered the value of r to 0.86. It is apparent that this drastic reduction in the protic character of the aqueous phase has reduced the sensitivity of the ether–water system to changes in lipophilicity of solutes by a factor of 2.8 (*i.e.*, 1.13/0.4). Diethylformamide, by disrupting the water envelope around a nonpolar solute, in all probability reduces the entropy factor in phase transfer.

The *intercept* value for each of the regression equations in Table VIII can be used as a measure of the lipophilicity of the solvent in a slightly different fashion. It is apparent that the intercept value in the equation for a given solvent system

Table IX

Relationship between Phenol Partition Coefficients in Octanol and Cyclohexane

Phenol	*Log* $P_{cyclohexane}$[a]	*Log* K_{HB}[b]	*Obsd*[c] *Log* $P_{octanol}$	*Calcd*[d] *Log* $P_{octanol}$	$\lvert\Delta \log P\rvert$
Unsubstituted	−0.85	0.00	1.46	1.50	0.04
4-Me	−0.14	−0.16	1.94	2.02	0.08
4-Et	0.40	−0.11	2.44	2.62	0.18
4-*tert*-Butyl	1.12	−0.27	3.31	3.15	0.17
3-F	−0.85[124]	0.39	1.93	1.97	0.04
4-F	−1.00	0.24	1.77	1.64	0.14
4-Cl	−0.70[124]	0.48	2.39	2.24	0.16
4-NO_2	−1.93	1.33	1.96	2.01	0.05
2,3-$(CH)_4$	0.52	0.16	2.98	3.06	0.08

[a] Some values are average of two determinations; see Table XVII. [b] From ref 117. [c] From ref 10 and 58. [d] Calculated using eq 34.

is the log P for any solute which is distributed equally between water and octanol; *i.e.*, $\log P_{octanol} = 0$. Thus a negative intercept for any equation indicates that the solvent is more lipophilic than octanol, and a positive intercept indicates that it is more hydrophilic. This is more readily apparent if one examines a homologous series of solutes, for example, the carboxylic acids. The octanol log P values begin at −0.54 for formic and rise to −0.17 for acetic and to +0.33 for propionic. Therefore, it takes between two and three lipophilic methylene groups to balance the hydrophilic carboxyl group and allow the octanol to share the solute equally with water.

In the oleyl alcohol–water system, it takes one *additional* methylene group before a carboxylic acid becomes lipophilic enough to be equally shared; *i.e.*, $\log P_{oleyl\ alc} = 0$ between propionic and butyric. Similarly, it is noted that in nitrobenzene–water it takes two *additional* methylenes, in benzene-water it takes three, and in CCl_4–water it takes about 4.5 additional groups to bring the solute to an equal lipophilic level with the organic phase.

Using the intercept values from the "A" or "sole" equation as a measure of the solvent's lipophilicity, we see that there is a very good correlation between these values and the water content at saturation.

$$\log (H_2O) = 1.077[\text{intercept}] + 0.249 \qquad (35)$$

n	r	s
17	0.979	0.217

Sometimes it may be misleading to think of a scale of "lipophilicity" as the simple reciprocal of a "hydrophilicity" scale, but eq 35 shows that the *inability* of a partition solvent to "accommodate" water is a good measure of its lipophilic behavior toward a great assortment of organic solutes.

A more complex kind of partition, but one which can be studied by means of linear regression equations similar to those in Table VIII, is that of the distribution of small organic molecules between proteins and an aqueous phase. A large number of such examples are known which can be correlated by an equation similar to eq 32.

$$\log K = a \log P + b \qquad (36)$$

In eq 36, K is an equilibrium constant measuring the binding of the small solute molecule by protein. In some work, the expression log (B/F) has been used instead of K. B represents the per cent of small molecules partitioned onto the protein, while F is the per cent of small molecule in the aqueous phase. A number of such examples are given in Table X.

In other examples the binding constant is expressed as $1/C$ where C is the molar concentration of small molecule necessary to produce a 1:1 (or higher, as indicated) complex of protein and small molecule.

The way the binding constant is defined greatly affects the intercepts listed in Table X so that only those defined in the same way can be compared. The slopes, however, differ very little regardless of the system, the type of compound studied, or the way in which the binding constant is defined.

Omitting the slopes for examples 1, 2, and 9 where the work was done at 4° (since it is known the slopes for the Hammett-type relationships are higher at lower temperatures), and omitting the rather deviant value of example 12, we are left with a set of 14 slopes with a mean value and standard deviation of 0.55 ± 0.06. This is amazingly constant considering the variations in conditions. The relationship between the results in Table X and those of Table VIII calls for further careful analysis. None of the slopes in Table VIII are as low as 0.54; the lowest for a carefully studied system is that of the butanols (0.72). In this sense, butanols behave more like the proteins than the other solvents of Table VIII. In fact, Scholtan[130] has shown that the binding of many drugs to serum protein follows the relationship

$$\log K = 0.9 \log P_{i\text{-BuOH}} + \text{constant} \qquad (37)$$

In eq 37, there is almost a 1:1 relationship between the logarithms of the two kinds of equilibrium constants. In this limited sense butanol, saturated with water, resembles a protein in structure.

Of course, in actual fact, saturated butanol which contains a greater number of water molecules than butanol molecules, is not at all like a protein. If the main driving force in the transfer from water into octanol or onto a protein is desolvation of the water about the solute, then we can postulate that the degree of desolvation must be about the same in each process. In the case of butanol, the solute molecule, in entering the butanol phase, finds itself in a rather aqueous environment. While the structure of the "flickering clusters" around the solute must be largely broken up in butanol, more such structures must be present than in solvents such as octanol or benzene. In the case of the proteins of Table X, since the weighting factor with the $\log P_{octanol}$ term is 0.5, one could postulate that only half as much desolvation occurs on the average in partitioning onto a protein as into octanol; that is, for a given increment in hydrophobicity (say, a phenyl group), the driving force for partitioning onto protein is only half of that of partitioning into octanol. One way of rationalizing this is to postulate that the solute molecules are partitioned onto the *surface* of the protein and in this way only partially desolvated. This seems a more logical explanation than to assume that they are completely engulfed by protein

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(127) A. E. Bird and A. C. Marshall, *Biochem. Pharmacol.*, **16**, 2275 (1967).
(128) C. Hansch and F. Helmer, *J. Polym. Sci., Part A-1*, **6**, 3295 (1968).
(129) J. M. Vandenbelt, C. Hansch, and C. Church, unpublished results.
(130) W. Scholtan, *Arzneim.-Forsch.*, **18**, 505 (1968).

Table X

Partitioning of Organic Compounds between Proteins and Aqueous Phases

Type of compound	*Macromolecule*[a]	K^b	*a*	*b*	*n*	*r*	*s*	*Ref*	*T*, °C
1. Miscellaneous	BSA (1:1)	1/*C*	0.75	2.30	42	0.960	0.159	9	4
2. Miscellaneous	BSA (3:1)	1/*C*	0.59	2.03	16	0.900	0.133	9	4
3. Barbiturates	BSA (1:1)	1/*C*	0.58	2.40	4	0.961	0.137	9	RT
4. Barbiturates	BSA	B/F	0.51	−1.22	17	0.896	0.181	126	RT
5. RCOO−	BSA	*K*	0.59[c]	−6.51	5	0.966	0.213	9	23
6. Miscellaneous	BSA (1:1)	1/*C*	0.67	2.48	25	0.945	0.242	129	37
7. Penicillins	Human serum	B/F	0.49[c]	−0.63	79	0.924	0.134	127	~22
8. Thyroxine analogs	Albumin	*K*	0.46[c]	2.59	8	0.950	0.237	126	37
9. Miscellaneous	Hemoglobin	1/*C*	0.71	1.51	17	0.950	0.160	9	4
10. ROH	Ribonuclease	*K*	0.50	−1.56	4	0.999	0.012	9	62
11. Acetamides	Nylon	*K*	0.69	−7.16	7	0.961	0.203	128	26.5
12. Acetanilides	Rayon	*K*	0.84	−7.24	7	0.967	0.227	128	26.5
13. Barbiturates	Liver[d]	B/F	0.52	−1.14	5	0.973	0.124	126	RT
14. Barbiturates	Heart[d]	B/F	0.62	−1.48	5	0.950	0.207	126	RT
15. Barbiturates	Kidney[d]	B/F	0.53	−1.42	5	0.962	0.152	126	RT
16. Barbiturates	Lung[d]	B/F	0.56	−1.50	5	0.956	0.173	126	RT
17. Barbiturates	Brain[d]	B/F	0.52	−1.44	5	0.973	0.125	126	RT
18. Barbiturates	Muscle[d]	B/F	0.48	−1.45	5	0.970	0.121	126	RT

[a] BSA = bovine serum albumin. [b] *C* = molar concentration; B/F = ratio bound to free; for definition of *K*, see original article. [c] π values used instead of log *P*. [d] Homogenized.

(as they are in passing into butanol) but that the "sweater" of outer molecules is not completely stripped from the solute.

There are instances in which the slope relating binding to $\log P_{octanol}$ is 1. For example, the correlation of $\log 1/K_m$ with log *P* for chymotrypsin substrates[131] and inhibitors is essentially 1 for substituents thought to be binding in the ρ_2 area. K_m is the Michaelis constant and is an approximate binding constant. Chymotrypsin is known to contain a deep cleft which may constitute the ρ_2 area and, in this instance, complete desolvation of the substituent may occur.

V. Additive-Constitutive Properties

It was apparent to Meyer[25] and Overton,[26] as well as the other early workers in the field, that in a homologous series the partition coefficient increased by a factor of from 2 to 4 per CH_2. Cohn and Edsal[102] verified that this kind of additivity held for the solubility ratios of amino acids in ethanol and water. They also extended it to include values for the groups $-CH_2CONH-$, OH, SH, and C_6H_5, and for dipolar ionization. Collander[4] determined that $\Delta P/CH_2$ fell in the range of 2 to 4 for the ether–water system and 1.8 to 3.0 for the butanol–water system. He also reported a range of values for ΔP when the following substitutions were made: OH for H, NH_2 for H, CO_2H for CH_3, CO_2H for $CONH_2$, and halogens for H. In view of these long-standing observations, it is surprising that no really systematic effort was made to study the additive character of the partition coefficient until the early 60's.

A. DEFINITION OF π

Additivity was first established for a wide variety of groups in a study of the substituent constant, π, defined[10] in an analogous fashion to the Hammett σ constant

$$\pi_X = \log P_X - \log P_H$$

where P_X is the derivative of a parent molecule, P_H, and thus π is the logarithm of the partition coefficient of the function X. For example, π_{Cl} could be obtained as follows.

$$\pi_{Cl} = \log P_{chlorobenzene} - \log P_{benzene}$$

(131) C. Hansch and E. Coats, *J. Pharm. Sci.*, 59, 731 (1970).

B. SUBSTITUENT FREE ENERGIES AND INTERACTION TERMS

It has been found that π values are relatively constant from one system to another as long as there are no special steric or electronic interactions of the substituents not contained in the reference system. For example, it has been found that π_{CH_3} for groups attached to various benzene derivatives has a value in the octanol–water system of 0.50 ± 0.04 for 15 different examples. The weak interaction of the methyl group with functions as active as a nitro group is exceptional. Most other π values are not so constant with respect to electronic environment. For example, in 15 examples of π_{NO_2} in aromatic systems, π had a mean value and standard deviation of 0.01 ± 0.32.

The function π is best viewed in extrathermodynamic terms. The symbols H-N-H and X-N-H can be used to represent a solute nuclei (N), the first one unsubstituted and the other containing the substituent X. The parameter π can then be defined by a comparison of two equilibria

$$\overset{H}{\text{H-N-H}} \underset{}{\overset{K_1}{\rightleftharpoons}} \overset{L}{\text{H-N-H}} \quad K_1 = (\text{H-N-H})^L/(\text{H-N-H})^H$$

$$\overset{H}{\text{X-N-H}} \underset{}{\overset{K_2}{\rightleftharpoons}} \overset{L}{\text{X-N-H}} \quad K_2 = (\text{X-N-H})^L/(\text{X-N-H})^H$$

The superscripts H and L denote the hydrophilic (H_2O) and lipophilic (solvent) phases and refer to the phase in which the molecule is located.

$$\pi = \log K_2/K_1$$

That is, the ratio of the equilibrium constants is equivalent to the equilibrium constant for the reaction

$$\text{X-N-H}^H + \text{H-N-H}^L \rightleftharpoons \text{X-N-H}^L + \text{H-N-H}^H \quad (38)$$

The free energy change resulting from the introduction of X on the first of the above equilibria would be

$$2.3RT \log K_2/K_1 = G_{X-N-H}{}^{L} + G_{H-N-H}{}^{H} - G_{X-N-H}{}^{H} - G_{H-N-H}{}^{L} \quad (39)$$

If we assume that the free energy of an individual molecule in eq 38 can be represented as the sum of its parts and their *interaction*, we may write

$$G_{X-N-H}{}^{L} = G_{X}{}^{L} + G_{N}{}^{L} + G_{H}{}^{L} + G_{XN}{}^{L} + G_{HN}{}^{L} + G_{XH}{}^{L} \quad (40)$$

In eq 40, the terms on the right represent the free energies of the substituents X or H and their interactions with the basic structure N ($G_{XN}{}^{L}$) or each other ($G_{XH}{}^{L}$). Formulating the other molecules in this fashion and substituting into eq 39 yields

$$2.3RT \log K_2/K_1 = G_{X}{}^{L} + G_{XN}{}^{L} + G_{XH}{}^{L} + G_{H}{}^{H} + G_{HN}{}^{H} + G_{HH}{}^{H} - G_{X}{}^{H} - G_{XN}{}^{H} - G_{XH}{}^{H} - G_{H}{}^{L} - G_{HN}{}^{L} - G_{HH}{}^{L} \quad (41)$$

Making substitutions of the type $G_{X}{}^{L} - G_{X}{}^{H} = \Delta G_X$, eq 41 is converted to

$$2.3RT \log K_2/K_1 = \Delta G_X + \Delta G_{XN} + \Delta G_{XH} - \Delta G_H - \Delta G_{HN} - \Delta G_{HH} \quad (42)$$

If the interaction terms can be neglected, then

$$\pi = 2.3RT \log K_2/K_1 = \Delta G_X - \Delta G_H \quad (43)$$

When two functions are involved, the following equilibria must be considered.

$$\text{H-}\overset{\text{H}}{\text{N}}\text{-Y} \overset{K_3}{\rightleftharpoons} \text{H-}\overset{\text{L}}{\text{N}}\text{-Y} \quad (44)$$

$$K_3 = (\text{H-N-Y})^L/(\text{H-N-Y})^H$$

$$\text{X-N-Y} \overset{K_4}{\rightleftharpoons} \text{X-N-Y} \quad (45)$$

$$K_4 = (\text{X-N-Y})^L/(\text{X-N-Y})^H$$

Equation 46 can then be derived from eq 44 and 45.

$$\pi = 2.3RT \log K_4/K_3 = \Delta G_X + \Delta G_{XN} + \Delta G_{XY} - \Delta G_{HY} - \Delta G_H - \Delta G_{HN} \quad (46)$$

Subtracting eq 43 from 46 yields

$$\Delta\pi = \Delta G_{XY} + \Delta G_{HH} - \Delta G_{HY} - \Delta G_{XH} \quad (47)$$

For $\Delta\pi$ to equal or approach 0, the four interaction terms must be equal to or approach 0. (There is of course the unlikely case where they might cancel each other so that $\Delta\pi = 0$.) As the number of changes in the systems under comparison becomes larger, so do the interaction terms, and hence the possibility that π from very different systems will remain constant becomes less likely. It is apparent from this analysis that the approach of Cratin[61] (see section II.C) cannot be extended indefinitely and that, for the present, one is limited to the use of model systems working outside of classical thermodynamics.

It has been shown[10] that the difference in π constants from two different systems is highly dependent on electronic interactions. This is illustrated by eq 48–51 in which the Hammett function,[109] σ, is the measure of electronic interaction. A good correlation is obtained with phenols in eq 48. The positive coefficient with σ indicates that an electron-withdrawing substituent, X, will be relatively better accommodated by octanol when it is moved from benzene to phenol. Surprisingly enough, a poorer correlation is obtained using σ^-. The reason for this may be that the linear relationship between $\Delta\pi$ and σ does not cover a very wide range of σ values. For example, placing two nitro groups on phenol yields a negative $\Delta\pi$ rather than a positive $\Delta\pi$ obtained for mononitro functions in eq 48.

Equation	n	r	s	
$\Delta\pi = \pi_{\text{phenol}} - \pi_{\text{benzene}} = 0.82\sigma + 0.06$	24	0.954	0.097	(48)
$\Delta\pi = \pi_{\text{benzyl alc}} - \pi_{\text{benzene}} = 0.47\sigma + 0.04$	11	0.937	0.086	(49)
$\Delta\pi = \pi_{\text{phenoxyacetic acid}} - \pi_{\text{benzene}} = 0.36\sigma + 0.04$	22	0.754	0.100	(50)
$\Delta\pi = \pi_{\text{nitrobenzene}} - \pi_{\text{benzene}} = -0.51\sigma + 0.28$	20	0.676	0.250	(51)

1. Inductive Effect

Relatively little systematic effort has been expended studying systems in which the inductive effect of one substituent on another can be cleanly dissected away from other effects.

It is clear in the benzyl alcohols correlated by eq 49 that electron-withdrawing substituents increase log P values relative to benzene. For example

$$\pi_{NO_2} = \log P_{\text{nitrobenzene}} - \log P_{\text{benzene}} = -0.28$$

$$\pi_{NO_2} = \log P_{\text{4-nitrobenzyl alc}} - \log P_{\text{benzyl alc}} = 0.11$$

In this example it seems unlikely that the primary effect on π is the action of CH_2OH on NO_2; it seems more reasonable to assume that the electron-withdrawing action of NO_2 on the region near the OH function is responsible for $\Delta\pi$ of 0.39. The inductive effect of the nitro group which is insulated from the OH by the CH_2 unit is apparently making the lone-pair electrons of the OH function less available for hydrogen bonding lowering the affinity of this function for the water phase. This same effect is quite apparent with anilines and phenols bearing electron-withdrawing functions. While the inductive withdrawal of electrons from the region of a function containing lone-pair electrons often raises its π value, this is not always so. π_{Cl} from the benzene system is 0.71, while $\pi_{4\text{-Cl}}$ in the nitrobenzene system is only 0.54, and $\pi_{3\text{-Cl}}$ is 0.61.

That the inductive effect is quite small with alkyl groups is illustrated by eq 52 and 53.

$$\pi_{CH_2} = \log P_{EtNO_2} - \log P_{MeNO_2} = 0.18 - (-0.33) = 0.51 \quad (52)$$

$$\pi_{CH_2} = \log P_{PrNO_2} - \log P_{EtNO_2} = 0.65 - 0.18 = 0.47 \quad (53)$$

2. Resonance Effect

The effect of electron delocalization on π values is well illustrated by the difference between aliphatic and aromatic π values shown in Table XI. The effect of moving functions from aliphatic to aromatic positions is a complex one. The amino group stands out by showing the smallest change, this despite the fact that a large amount of evidence leaves no doubt about the delocalization of the nitrogen lone-pair electrons. The higher π value which should result from this effect is apparently offset by better hydrogen bonding of the two hydrogen atoms which increases affinity for the water phase. When the hydrogen atoms are removed, as in the $N(CH_3)_2$ function, we see the expected $\Delta\pi$ value, that is, one somewhat higher than $\Delta\pi_{OCH_3}$. With the more electronegative oxygen atom this effect is not observed. The largest $\Delta\pi$ is for NO_2, and it appeared possible that the acidity of the α-hydrogen atoms might be playing a role in conferring unusual hydrophilic character to the aliphatic nitro solutes. However, π_{NO_2} was found to be essentially unchanged for the *tert*-nitro derivative, 2-methyl-2-nitropropane.

Table XI

Comparison of Aromatic and Aliphatic π Values

Function	*Aromatic* π *Log* $P_{C_6H_5X}$ − *log* $P_{C_6H_6}$	*Aliphatic* π *Log* P_{RX} − *log* P_{RH}	$\Delta\pi$ $\pi_{ar} - \pi_{al}$
NH_2	−1.23	−1.19	−0.04
I	1.12	1.00	0.12
S-CH_3	0.61	0.45	0.16
$COCH_3$	−0.55	−0.71	0.16
$CONH_2$	−1.49	−1.71	0.22
$COOCH_3$	−0.01	−0.27	0.26
Br	0.86	0.60	0.26
CN	−0.57	−0.84	0.27
F	0.14	−0.17	0.31
Cl	0.71	0.39	0.32
COOH	−0.28	−0.67	0.39
OCH_3	−0.02	−0.47	0.45
OC_6H_5	2.08	1.61	0.47
$N(CH_3)_2$	0.18	−0.30	0.48
OH	−0.67	−1.16	0.49
NO_2	−0.28	−0.85	0.57

With the exception of NH_2, transferring any function from an aliphatic to an aromatic position results in an increase in lipophilicity. Actually, $\Delta\pi$ for NH_2 is so small that it can be considered to be 0.

Replacing a single bond with a double bond results in a constant $\Delta\pi$ of about −0.3. This can be illustrated as follows by comparing $\pi_{-CH_2CH_2-}$ (=1.00) with $\pi_{-CH=CH-}$ derived from five systems (Chart I). If, indeed, log P or π is primarily determined (in apolar functions) by the removal of an envelope of structured water molecules, then it is not surprising that $\pi_{-CH=CH-}$ is the same in one of the conjugated double bonds in naphthalene as in an isolated double bond in 5-hexen-2-one.

Chart I

$\pi_{-CH=CH-} = \log P_{CH_3COCH_2CH_2CH=CH_2} - \log P_{CH_3COCH_2CH_3} = 1.02 - 0.29 =$ 0.73

$\pi_{-CH=CH-} = {}^1/_3 \log P_{benzene} = {}^1/_3(2.13) =$ 0.71

$\pi_{-CH=CH} = {}^1/_5 \log P_{naphthalene} = {}^1/_5(3.45) =$ 0.69

$\pi_{-CH=CH} = \log P_{C_6H_5OCH_2CH=CH_2} - \log P_{C_6H_5OCH_3} = 2.94 - 2.11 =$ 0.83

$\pi_{-CH=CH-} = {}^1/_2(\log P_{diallyl} - 1.00) = {}^1/_2(2.45 - 1.00) =$ 0.72

Av = 0.73

$\Delta\pi$ = −0.27

An acetylenic group has a somewhat lower π value.

$$\pi_{-C\equiv CH} = \log P_{1\text{-pentyne}} - \log P_{C_3H_8} = 1.98 - 1.50 = 0.48$$

$$\pi_{-C\equiv CH} = \log P_{C_6H_5C\equiv CH} - \log P_{C_6H_6} = 2.53 - 2.13 = 0.40$$

Conjugation of π-electron systems does not appear to result in big changes in π values even when a heteroatom is included in the system. Table XII illustrates the amount of variance in $\pi_{-CH=CHCH=CH-}$ in a variety of different aromatic systems. The mean value and standard deviation for the 10 systems is 1.38 ± 0.036.

Table XII

Constancy of π for -CH=CHCH=CH-

	$\pi_{-CH=CHCH=CH-}$
Log P_{indole} − log $P_{pyrrole}$ = 2.14 − 0.75 =	1.39
Log $P_{quinoline}$ − log $P_{pyridine}$ = 2.03 − 0.65 =	1.38
log $P_{isoquinoline}$ − log $P_{pyridine}$ = 2.08 − 0.65 =	1.43
Log $P_{acridine}$ − log $P_{quinoline}$ = 3.40 − 2.03 =	1.37
Log $P_{dibenzofuran}$ − log $P_{benzofuran}$ = 4.12 − 2.67 =	1.45
Log $P_{benzothiophene}$ − log $P_{thiophene}$ = 3.12 − 1.81 =	1.31
Log $P_{naphthalene}$ − log $P_{benzene}$ = 3.45 − 2.13 =	1.32
${}^2/_3$ log $P_{benzene}$ = ${}^2/_3$(2.13) =	1.42
Log $P_{\beta\text{-naphthol}}$ − log P_{phenol} = 2.84 − 1.46 =	1.38
Log $P_{\beta\text{-naphthoxyacetic acid}}$ − log $P_{phenoxyacetic acid}$ = 2.54 − 1.21 =	1.33
Av =	1.38 ± 0.036

3. Steric Effect

Steric effects can be quite varied in nature. The shielding of lone-pair electrons by inert alkyl groups produces a significant increase in π values.

$$\pi_{CH_3} = \log P_{2\text{-methylphenoxyacetic acid}} - \log P_{POA} = 2.10 - 1.26 = 0.84$$

$$\pi_{CH_3} = \log P_{3\text{-methylphenoxyacetic acid}} - \log P_{POA} = 1.78 - 1.26 = 0.52$$

Shielding a hydroxyl function by inert groups such as 2,6-substituted phenols reduces hydrogen bonding and results in a positive $\Delta\pi$. This is most pronounced in the case of a nonpolar solvent system such as cyclohexane.[132,133]

Crowding of functions may also reduce hydrophobic bonding with the opposite effect on $\Delta\pi$. For example, pentachlorophenol has a measured log P of 5.01, while its calculated value would be

$$\log P = \text{phenol} + 2\pi_{o\text{-Cl}} + 2\pi_{m\text{-Cl}} + \pi_{p\text{-Cl}} = 1.46 + 1.38 + 2.08 + 0.93 = 5.85$$

Assuming electronic effects of each Cl atom to be contained in the corresponding π_{Cl} value, $\Delta\pi_{steric} = 5.01 - 5.85 = 0.84$. Presumably, this would be the result of fewer water

(132) C. Golumbic, M. Orchin, and S. Weller, *J. Amer. Chem. Soc.*, 71, 2624 (1949).
(133) J. Fritz and C. Hedrick, *Anal. Chem.*, 37, 1015 (1965).

molecules clustered around each chlorine atom in the pentachloro derivative than in the monochloro derivatives.

1,2,3-Trimethoxybenzene is an interesting example of how the steric effect can operate to inhibit resonance and thus decrease π.

$$\log P_{C_6H_3(OCH_3)_3} = \log P_{C_6H_6} + 3\pi_{OCH_3} = 2.13 - 0.06 = 2.07$$

The measured value is 1.53, indicating greater than expected affinity for the water phase. If we assumed that only the central OCH_3 is perturbed and that it is twisted out of the plane of the ring so that resonance between the oxygen lone pair electrons and the π electrons of the benzene ring is prevented, then the central OCH_3 might be expected to have the π value of an aliphatic function. This can be tested as follows.

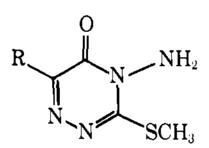
$$\pi_{OCH_3} = \log P_{1,2,3\text{-trimethoxybenzene}} - \log P_{1,3\text{-dimethoxybenzene}} = 1.53 - 2.09 = -0.56$$

The π value for the "twisted -OCH_3" (−0.56) is much closer to that of an aliphatic OCH_3 (−0.47) than it is to an ordinary aromatic -OCH_3 (−0.02).

Sometimes the steric effects of alkyl functions on the solubility characteristics of an adjacent carbonyl function can be quantitatively correlated with the Taft E_s parameter. The partition coefficients of a series of 2-alkyltriazinones are listed in Table XIII along with E_s values. The calculated log P values

Table XIII

Steric Effect in Triazinones



No.	R	Calcd log P^a	E_s	Obsd log P	Log P pred by eq 54	Obsd − pred
1.	CH_3	−0.16	0.00	−0.16	−0.14	−0.02
2.	C_2H_5	0.34	−0.07	0.46	0.41	0.05
3.	n-C_3H_7	0.84	−0.36	0.93	1.04	−0.11
4.	i-C_3H_7	0.64	−0.47	1.01	0.88	0.13
5.	i-C_4H_9	1.14	−0.93	1.39	1.57	−0.18
6.	*tert*-C_4H_9	0.94	−1.54	1.70	1.60	0.10
7.	i-C_5H_9	1.65	−0.35	1.85	1.85	0.00
8.	c-C_6H_{11}	1.81	−0.79	2.14	2.19	−0.05
9.	n-C_6H_{13}	2.35	−0.40	2.68	2.59	0.08

^{a} The methyl derivative used as the "parent" compound and π_{alk} from either the phenoxyacetic acid or benzene systems used to calculate the "normal" log P values of the remaining compounds.

are those expected from the addition of π_{alkyl} to unsubstituted triazinone. It is apparent that the observed values of Draber, Büchel, *et al.*,[134] are higher. Equation 54 rationalizes this difference in terms of E_s.

$$\log P_{obsd} = 1.026 \log P_{calcd} - 0.392E_s + 0.024 \quad (54)$$

n	r	s
9	0.993	0.018

Another instance in which chain branching results in hydrophilic shielding and increases log P (contrary to an expected negative $\Delta\pi$ as explained in the following section) has been reported[135] in the study of a series of dialkylphosphorodithiotic acids. Branching apparently also increases the acid dissociation constant, an effect which would not be expected from electronic forces alone.

Steric shielding of a tertiary nitrogen apparently explains the difference in the partition coefficients between the allo (planar and hindered access to N) and epiallo (N exposed at "bend") isomers of corynantheidine-type alkaloids.[136] In the heptane–water system, the $\Delta\pi$ for the allo–epiallo transition is +1.07 in one instance and +0.76 in another. However, it is not clear from the proposed structural formulas why there should be a much lower $\Delta\pi$ comparing the normal (planar) with the pseudo (nonplanar) in two other examples [$\Delta\pi$(speciogynine − mitrociliatine) = +0.11; $\Delta\pi$(dihydrocorynanthine − hirsutine) = +0.11].

Some care must be exercised in deciding whether a difference in observed partition coefficients between stereoisomers is truly the result of the balance of hydrophilic–lipophilic forces. For example, P values have been measured[137] in benzene–water for the exo (P = 2.37) and endo (P = 4.23) epimers of an analog of meperidine. However, the aqueous phase was buffered at 7.4 and, since the exo form is more basic (pK_a = 8.35 *vs.* 8.19), there is a lower percentage in the un-ionized form. The corrected P values are exo = 29 and endo = 30. The observed lower biological activity of the exo epimer stems from its pK_a.

4. *Branching*

A normal aliphatic chain usually has a higher π value than a branched chain. For example, $\pi_{3\text{-Pr}}$ = 1.45 and $\pi_{3\text{-}i\text{-Pr}}$ = 1.33 in the phenoxyacetic acid system. When branching occurs at the functional group, the effect appears to be slightly greater; *e.g.*, *tert*-BuOH = 0.37, 2-BuOH = 0.61, and 1-BuOH = 0.88. Similarly, log $P_{i\text{-PrNH}_2}$ = 0.03 while log P_{PrNH_2} = 0.31. In contrast to this, however, there seems to be no difference between log P for isopropylbenzene and propylbenzene. Also, there appears to be no lowering of log P in *tert*-butylbenzene. The observed value of 4.11 is what would be expected for the n-butyl derivative if calculated from the value of 3.68 for propylbenzene. Accepting the fact that some discrepanices remain to be resolved, we have, for the purpose of calculating log P values, tentatively used the value of −0.20 for branching.

5. *Conformational Effects*

Another problem which must be taken into account in the additive–constitutive character of log P is the conformation of organic compounds in solution. It might be expected that when aliphatic chains become long enough, they would tend to coil up in solution with the formation of molecular oil droplets. With simple molecules such as monofunctional straight-chain aliphatic compounds, clear-cut evidence seems to be lacking for such "balling-up" of chains. In fact, it ap-

(134) W. Draber, K. Büchel, K. Dickore, A. Trebst, and E. Pistorius, *Progr. Photosyn. Res.*, **3**, 1789 (1969).

(135) R. Zucal, J. Dean, and T. Handley, *Anal. Chem.*, **35**, 988 (1963).

(136) A. Beckett and D. Dwuma-Badu, *J. Pharm. Pharmacol.*, **21**, 162S (1969).

(137) P. Portoghese, A. Mikhail, and H. Kupferberg, *J. Med. Chem.*, **11**, 219 (1968).

pears that it will be quite difficult to disentangle this phenomenon from that of premicellular interactions.

If "balling-up" of an aliphatic chain occurred, one would expect the number of water molecules held in the flickering cluster around such a ball to be much less than the number held around the extended chain. This would mean a lower desolvation energy on phase transfer and, hence, a lesser increment in partition coefficient—possibly an abrupt discontinuity in $\Delta \log P$ as one ascends a homologous series.

A clear example of such changes in partition coefficient as one ascends a homologous series is lacking. In the RCOOH series, normal behavior occurs up to decanoic acid.

$$\text{av } \pi/CH_2 = {}^1/_8(\log P_{C_9H_{19}COOH} - \log P_{CH_3COOH}) = 0.53$$

However, $\Delta\pi$ between decanoic and dodecanoic acid is much smaller than the 1.0 unit expected in terms of simple additvity. The log P values for dodecanoic acid were determined using ^{14}C-labeled material. Great difficulty was experienced in obtaining reproducible results, and considerable uncertainty surrounds the value of 4.20 for dodecanoic acid. Whether this unexpectedly low value is due to a folding up of the aliphatic chain or a premicellular tail-to-tail dimerization remains an open question. Other solvent systems also produce a constant increment in log P per $-CH_2-$ group for fatty acid homologs.[138] This increment is about 0.6 in the heptane–water system for valeric through myristic acids.[139]

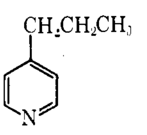
The alcohol homologous series also shows the expected increase in log P with the addition of each CH_2 unit. In this series

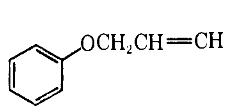
$$\text{av } \pi/CH_2 = {}^1/_{11}(\log P_{\text{dodecanol}} - \log P_{\text{methanol}}) = 0.52$$

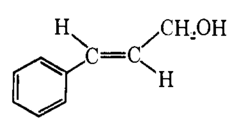
there was some difficulty in obtaining constant log P values over a wide concentration range for alcohols of greater chain length than C_{12}.

In summary, it would seem that "molecular oil droplet" formation does not occur with simple aliphatic compounds before C_{14}. If folding does not occur up to C_{14}, it would imply that there is an inherent stability in the aqueous phase of the aliphatic chain caused, perhaps, a by a restriction of rotation around each C–C bond as Aranow and Witten proposed.[79]

The situation is of course much different when more than one reactive center is present per molecule. It appears that folded conformations of many organic compounds in aqueous solution can be detected through partitioning studies. This is well illustrated by a study of derivatives of the type $C_6H_5CH_2CH_2CH_2X$. When X = H, log P was found to be 3.68 which is quite close to the calculated value: $\log P_{\text{benzene}} + 3\pi_{CH_2} = 2.13 + 3(0.50) = 3.63$. Other mixed aliphatic–aromatic compounds also give good agreement between calculated and observed values. However, in comparing π values







Obsd log P	2.10	2.94	1.95
Calcd log P	2.15	2.81	2.20

between RX and $C_6H_5(CH_2)_3X$, a constant discrepancy was observed as shown in Table XIV. The phenylpropyl functions

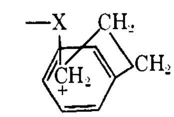
Table XIV

Effect upon π of Folding of Alkyl Chains

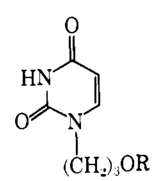
Function	$\pi_1{}^a$	$\pi_2{}^b$	$\pi_1 - \pi_2$
OH	−1.80	−1.16	0.64
F	−0.73	−0.17	0.56
Cl	−0.13	0.39	0.52
Br	0.04	0.60	0.56
I	0.22	1.00	0.78
COOH	−1.26	−0.67	0.59
$COOCH_3$	−0.91	−0.27	0.64
$COCH_3$	−1.26	−0.71	0.55
NH_2	−1.85	−1.19	0.66
CN	−1.47	−0.84	0.63
OCH_3	−0.98	−0.47	0.51
$CONH_2$	−2.28	−1.71	0.57
			Av = 0.60 ± 0.05

[a] $\log P_{C_6H_5(CH_2)_3X} - \log P_{C_6H_5(CH_2)_3H}$. [b] $\log P_{RX} - \log P_R$. R is a normal alkyl group of four carbon atoms or less.

turn out to have a greater affinity for the aqueous phase than one would expect from the corresponding aliphatic functions. Most surprising was the fact that $\Delta\pi$ for the two systems was essentially constant regardless of the kind of function compared. It was suggested that this greater than expected aqueous solubility of phenylpropyl derivatives is due to folding of the side chain onto the phenyl ring. Such folding could be caused by the interaction of the dipole of the side chain with the π electrons of the ring. It would also be promoted by intramolecular hydrophobic bonding. However, the dipolar interaction would appear to be critical in overcoming the small forces which tend to keep the chain extended since propylbenzene, lacking such a dipole, has the expected log P value. This compact form of the phenylpropyl derivative means a smaller apolar surface for solvation and, hence, a lower entropy change in the desolvation process of partitioning. Since the size or kind of polar function has little to do with $\Delta\pi$, it seems likely that this function projects away from the ring side-chain complex.



Nmr evidence has been gathered[140] to show that similar folding occurs in compounds having the following structure.



It has also been suggested[141] that such folding results in a lower than expected log P for vitamin K. Folding is included as one of the possible group interaction parameters for a π-additivity scheme developed for the cyclohexane–water system.[141]

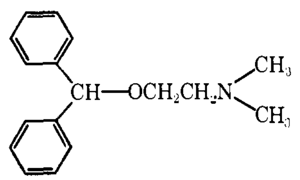
(138) A. Beckett and A. Moffat, *J. Pharm. Pharmacol.*, **21**, 144s (1969).

(139) D. Goodman, *J. Amer. Chem. Soc.*, **80**, 3887 (1958).

(140) B. Baker, M. Kawazu, D. Santi, and T. Schwan, *J. Med. Chem.*, **10**, 304 (1967).

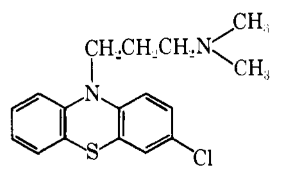
(141) D. Currie, C. Lough, R. Silver, and H. Holmes, *Can. J. Chem.*, **44**, 1035 (1966).

Certainly folding must be considered whenever a calculated log P must be used. The following two examples indicate how the problem can be treated in a straightforward manner.



diphenhydramine

Log P for diphenhydramine = 4.26 + 0.30 − 0.73 + 0.50 − 0.95 = 3.38, which would be adequate for most purposes, considering that the observed log P is 3.27. In the above example, 4.26 is 2(log $P_{C_6H_5}$). The value of 0.30 is for a CH_2 on which branching occurs. The value of (−0.73) for the OCH_2 moiety is obtained by subtracting 1.50 from 0.77, the value for log P_{EtOEt}. For the $-N(CH_3)_2$ unit we have used the value of −0.95 obtained for the solute, $C_6H_5(CH_2)_3N(CH_3)_2$. It is assumed that folding of diphenylhydramine occurs in aqueous solution, just as it did in the amine model system used in the calculations.



chlorpromazine

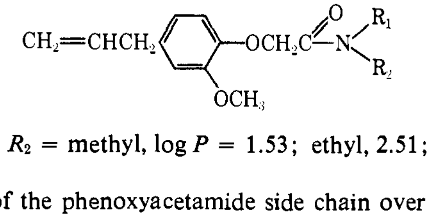
As another example log P for chlorpromazine can be calculated as 4.15 + 0.70 + 0.60 = 5.45, which is in satisfactory agreement with the observed log P = 5.35.

The value of 4.15 is log P for phenothiazine. To this is added π_{Cl} of 0.70 and 0.60 for $\pi_{(CH_2)_3N(CH_3)_2}$. For the side chain, π was calculated from a model in which the opportunity for folding was the same as for chlorpromazine.

$$\pi_{(CH_2)_3N(CH_3)_2} = \log P_{C_6H_5(CH_2)_3N(CH_3)_2} - \log P_{C_6H_6} = 2.73 - 2.13 = 0.60$$

The oleyl alcohol-water partition coefficients of a series of phenoxyacetamide derivatives[142] appear to provide further examples of folding over a benzene ring. In this case, the deviations from additivity in π values appear to be maximized when folding over the ring brings together hydrophobic portions of two para ring substituents.

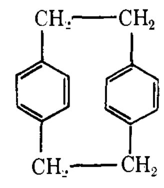
The basic structure investigated can be depicted as



When $R_1 = R_2$ = methyl, log P = 1.53; ethyl, 2.51; n-butyl, 1.80.

Folding of the phenoxyacetamide side chain over the benzene ring might be expected to show a constant $\Delta\pi$ as was indicated in the examples in Table XIV. But after the expected increase in log P in ascending the series from dimethyl to diethyl, a sudden *decrease* in lipophilic character is noted with the substituent chains of greater length. This observation can be explained if it is postulated that folding will occur in all cases, but if the alkyl chains, R_1 and R_2, are sufficiently long, they will be placed in such close proximity to the p-allyl group that cancellation of some hydrophobic character due to overlapping occurs.

Evidence that hydrophobic overlap can, indeed, lower the partition coefficient can be seen in molecules that are constrained to take an overlapped position. An example would be paracyclophane, whose log P would be expected to be close to twice that of xylene, if the entire hydrophobic area were exposed.



paracyclophane

The observed value as shown in Table XVII is even lower than that of xylene itself, and thus it appears that only one-half the potential hydrophobic area is "exposed."

Of course, we must assume that in all these determinations of P values care was taken to work below cmc. It is conceivable that if a constant solute concentration were employed throughout a homologous series, the cmc would be exceeded with the higher members, giving falsely low log P values for them. While part of the effect noted in the phenoxyacetamide series could have arisen from this cause, it is highly unlikely that *all* of it can be explained in this fashion, especially since the biological response of the series so closely follows the measured log P values.

Although an actual conformational change which brings a polar group on a side chain in close proximity with the π electron cloud on the ring seems the best way to explain these negative $\Delta\pi$'s (observed − calculated), nevertheless, there are some apparent weaknesses in this hypothesis. First of all, it seems entirely possible that the close approach of the polar group and the ring, which causes the hydrophobic chain to fold on itself, might eliminate a corresponding amount of *polar* bonding with water, and the loss in hydrophilic bonding might cancel the loss in hydrophobic bonding. Furthermore, the folding must occur in the aqueous phase to cause the unexpectedly low log P, but it is difficult to imagine any induced polar force or charge-transfer condition which would be effective in a medium as polar as water. Finally, once the initial π lowering is encountered in several homologous series, no additional effect is seen as the chain length is increased, even though a larger hydrophobic area is presumed to be coming into close contact. This is very apparent in a series of 3-substituted 2-hydroxynaphthoquinones[143] where the same $-\Delta\pi$ is noted whether the polar group and ring are separated by three methylene units or nine. Of course, in a chain longer than three carbon atoms, the entropy gained through hydrophobic overlap might be exactly cancelled by the energy needed to overlap the hydrogen atoms as each C–C bond is rotated in the manner needed for folding the chain.

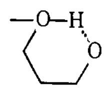
It is to be expected that solutes which can readily form intramolecular hydrogen bonds will adopt this favored con-

(142) T. Irikura, *Yakugaku Zasshi*, 82, 356 (1962).

(143) L. Fieser, M. Ettlinger, and G. Fawaz, *J. Amer. Chem. Soc.*, 70, 3228 (1948).

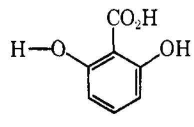
figuration during partitioning and that π additivity will certainly be affected. Salicylic acid provides a typical example.

$$\log P_{o\text{-hydroxybenzoic acid}} - \log P_{p\text{-hydroxybenzoic acid}} = \Delta\pi$$
$$2.21 \qquad 1.58 \qquad 0.63$$



The $\Delta\pi$ for a six-membered H-bonded ring is positive, as expected, because intramolecular H-bonding would reduce the affinity for the aqueous phase.

An even further reduction in hydrophobicity is possible when two ortho groups are involved:



$$\log P\text{ (calcd)} = \log P_{p\text{-hydroxybenzoic acid}} + \pi_{(\text{OH para to CO}_2\text{H})}$$
$$= 1.58 + (-0.30) = 1.28$$
$$\log P\text{ (obsd)} = 2.20$$
$$\Delta\pi = +0.92$$

An intramolecular H bond of the type (-N—H···O) in a six-membered ring is not expected to be as strong, and the $\Delta\pi$ is found to be smaller.

$$\log P_{\text{anthranilic acid}} - \log P_{p\text{-aminobenzoic acid}} = \Delta\pi$$
$$1.21 \qquad 0.68 \qquad = +0.53$$

VI. Uses of Partition Measurements

A. COUNTERCURRENT DISTRIBUTION

The relationship between the partition coefficient of a particular solute and the number of transfers necessary to properly characterize the distribution curve or to separate it from closely allied impurities is adequately covered in the literature.[22,106,144–147] It is a common practice to make a number of separate preliminary runs with both solute and suspected impurity in several solvent systems to attempt to optimize the two solvents used for the final distribution. Following the calculation procedures presented in section V and using the values listed in Table XVII as "parent" molecules, it may be possible to obtain reliable estimates of partition coefficients of a great number of solutes for many systems in which measurements have not yet been made. This procedure might considerably shorten the time required to find optimal extraction conditions. Furthermore, as more knowledge is gained on the effect of different solvents upon solute conformation (section V.D), better advantage could be taken in enhancing selectivity by providing an environment with precisely the right balance of conformational averages.[23] This knowledge might also prove helpful in predicting the possibility of metastable conformational forms which can cause an apparent shift in the partition ratio during fractionation.

B. MEASUREMENT OF EQUILIBRIA

The use of partitioning measurements to determine the equilibrium constants for the reactions

$$BH^+ \overset{aq}{\rightleftharpoons} B + H^+$$
$$HA \overset{aq}{\rightleftharpoons} H^+ + A^-$$
$$2HA \overset{org}{\rightleftharpoons} (HA)_2$$
$$HA + H_2O \rightleftharpoons HA\cdot H_2O\ (+\ (HA)_2\cdot H_2O + HA\cdot 2H_2O)$$

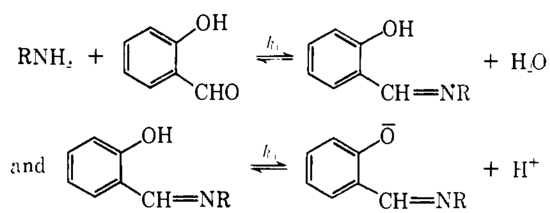
has been discussed in section II.B.

Many of the partition coefficient values reported in Table XVII for solutes which are metal ion complexing agents[50,148,149] have been measured in order to determine the equilibrium constant for the reaction of the type

$$M^{n+}{}_{(w)} + nH_2C_{(o)} \rightleftharpoons M(HC)_{n(o)} + nH^+{}_{(w)}$$

where M is the metal of valence n, H_2C is the neutral complexing agent (*e.g.*, dithiazone), and (w) and (o) refer to the water and organic phases, respectively.

Another type of equilibrium studied by partitioning methods is that between an aldehyde and amine in forming a Schiff base. With salicylaldehyde[150,151] a study of the distribution as a function of pH must take into consideration a second equilibrium



The shape of the curves depicting this relationship are seen in Figures 3 and 4. In each figure, section 1 of the curve represents the P value for free aldehyde, section 2 that of the Schiff base, and section 3 that of the phenoxide ion of the Schiff base. From separate evaluation of the dissociation constants of the components of the Schiff base, the log of the formation constant, log K_f, is calculated to be 4.75 for the *n*-butylsalicylidenimine and 4.57 for the methyl analog.

C. RELATIONSHIP TO HLB AND EMULSION SYSTEMS

The HLB (hydrophile–lipophile balance) system, which was established on a purely empirical basis,[152] has been a very potent tool in the hands of emulsion technologists, but it has been felt for some time that even more rapid strides could be made in this field if this system could be directly related to the partition coefficient which is in turn based firmly on thermodynamics. Experimental difficulties have made such a task very difficult,[153] but Davies, who studied the kinetics of coalescence in emulsion systems, has proposed an equation[154] which relates the two in simple fashion

$$(\text{HLB} - 7) = 0.36 \ln 1/P$$

From this relationship it appears possible to give extrathermodynamic significance to each structural element in deter-

(144) L. Craig, C. Golumbic, H. Mighton, and E. Titus, *J. Biol. Chem.*, **161**, 321 (1945).
(145) R. Priore and R. Kirdani, *Anal. Biochem.*, 24, 360 (1968).
(146) L. Craig, *J. Biol. Chem.*, **155**, 519 (1944).
(147) B. Williamson and L. Craig, *ibid.*, **168**, 687 (1947).
(148) S. Balt and E. Vandalen, *Anal. Chim. Acta*, **30**, 434 (1964).
(149) B. Hok, *Svensk Kem. Tidskr.*, **65**, 182 (1953).
(150) R. Green and P. Alexander, *Aust. J. Chem.*, **18**, 329 (1965).
(151) R. Green and E. Measurier, *ibid.*, **19**, 229 (1966).
(152) W. Griffin, *J. Soc. Cosmet. Chem.*, **1**, 311 (1949).
(153) W. Griffin, *ibid.*, **5**, 249 (1954).
(154) J. T. Davies, *Proc. Int. Congr. Surface Activ., 2nd*, **1**, 476 (1957).

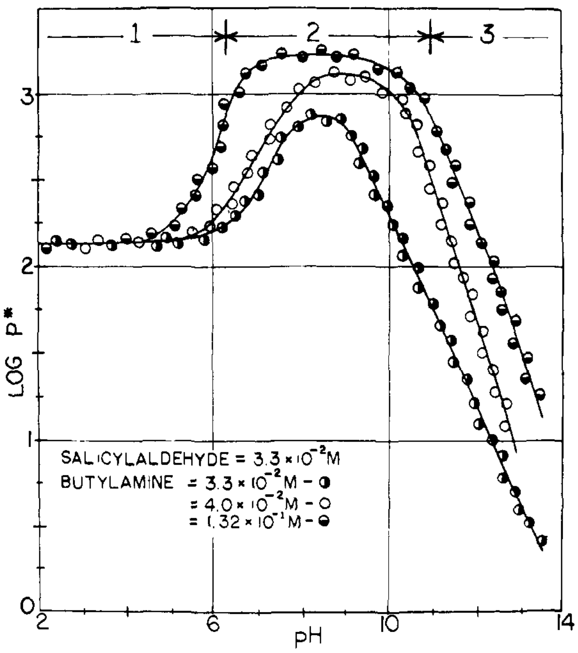


Figure 3. Formation of *n*-butylsalicylidenimine and partitioning between toluene and water.

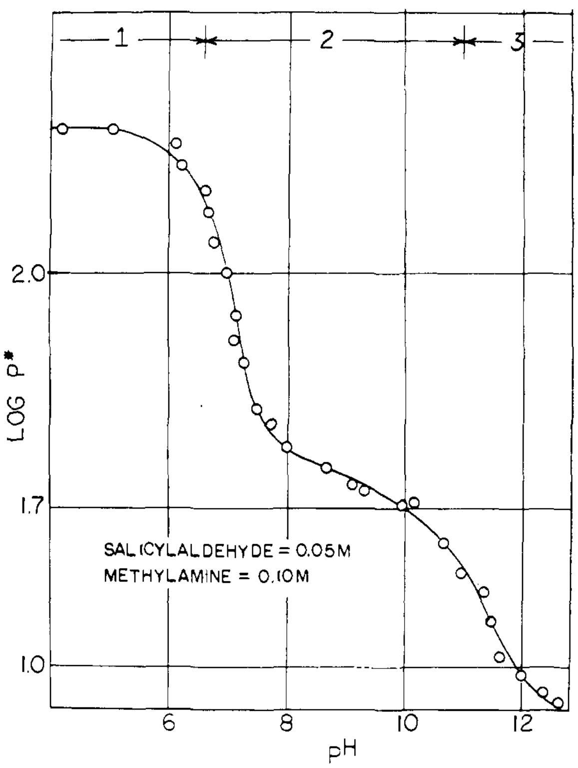


Figure 4. Formation of methylsalicylidenimine and partitioning between toluene and water.

mining the molecule's ability to function as a wetting agent, detergent, or defoamer.[61,155]

D. MEASUREMENT OF DISSOLUTION AND PARTITIONING RATE OF DRUGS

It is widely accepted that the dissolution rate of any drug given in solid form can have a marked influence upon the amount effectively absorbed. Since drug absorption is also affected by its effective partition coefficient, it is desirable to measure these properties simultaneously. This becomes more important in view of the observation that some surfactants are capable of increasing the rate of solution while simultaneously lowering the rate of partitioning.[156] With drugs that are poorly water soluble, the usual measurements of solubility rates require large volumes of water so that the drug concentration is far below the saturation level. Yet this often means that a separate extraction step must be carried out so that a sufficiently high concentration of drug is obtained for accurate analysis.

As a model system, hard, nondisintegrating tablets of salicylic acid of uniform surface areas were stirred under standard conditions in aqueous buffer (pH 2) with an upper octanol phase present.[156] The system can be described as follows.

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C}$$

A = weight of drug in tablet form, B = weight of drug in aqueous phase, C = weight of drug in octanol phase; then if W_s = weight of drug needed to saturate the aqueous phase, and using equal volumes of the two phases, the kinetic equations are

$$-\mathrm{d}A/\mathrm{d}t = k_1(W_s - B)$$

$$\mathrm{d}B/\mathrm{d}t = k_1(W_s - B) - k_2B$$

$$\mathrm{d}C/\mathrm{d}t = k_2B$$

In the early stages of dissolution, $W_s \gg B$ and

$$-\mathrm{d}A/\mathrm{d}t = k_1W_s \qquad (55)$$

Furthermore, for lipophilic drugs, a steady-state concentration of B is quickly attained

$$\mathrm{d}B/\mathrm{d}t = 0 = k_1(W_s - B) - k_2B \qquad (56)$$

and

$$\mathrm{d}C/\mathrm{d}t = k_2B = k_1(W_s - B) = -\mathrm{d}A/\mathrm{d}t \qquad (57)$$

The rate of appearance of drug in the lipid phase is easily measured and becomes equal to the dissolution rate in the aqueous phase.

If partitioning between aqueous and organic phases is to serve as a model system of how a biologically interesting solute passes through membranes in living tissue, then the *rate* at which equilibrium is attained might be as important as the equilibrium value itself. For solutes of similar structure, the activation energies for phase transfer are often approximately equal, and therefore the transfer rate constants are proportional to the equilibrium constants, P.[92] However, an interesting exception was reported[94] when a more rapid rate of partitioning from water to butanol was found for KCl than for NaCl, even though their P values are approximately equal. The measured difference in activation energy between these salts was 0.8 kcal/mol, which probably was due to

(155) P. Becher, "Emulsions, Theory and Practice," Reinhold, New York, N. Y., 1966, p 233.

(156) P. J. Niebergall, M. Patil, and E. Sugita, *J. Pharm. Sci.*, **56**, 943 (1967).

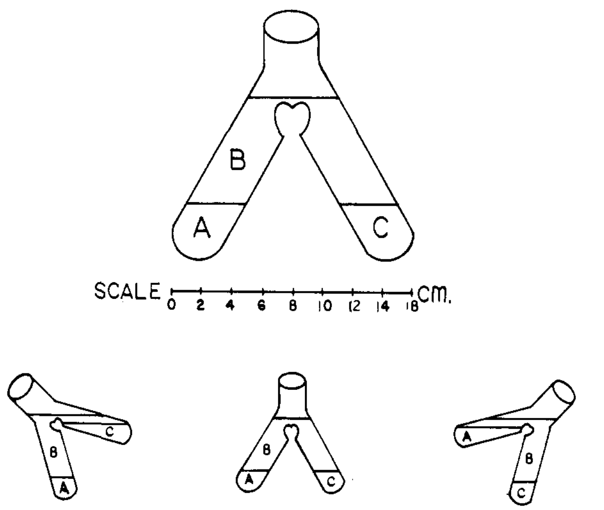


Figure 5. Effects of gentle rocking on the interfaces. Partitioning rate apparatus: Doluisio and Swintosky Y-tube.

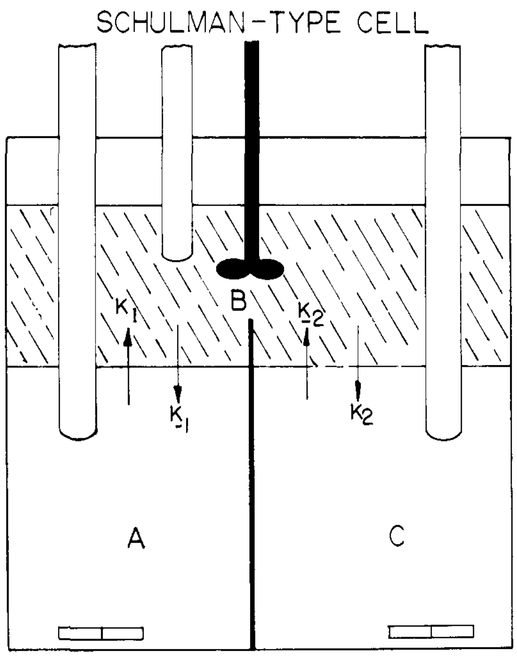


Figure 6. Magnetic stirrers used to study rate of transport across lipoid barrier; A, B, and C have the same meaning as in Figure 5.

differences in the loss of hydration as the ions entered the butanol phase.

Two basically different types of apparatus have been designed for partitioning rate studies. Doluisio and Swintosky[157] employed an inverted Y tube in which the oil phase in the neck was the only connecting "link" between the separate aqueous phases in the arms (see Figure 5). A gentle rocking motion was applied which gradually expanded and contracted the interfaces. This accelerated solute transfer but normally was insufficient to cause emulsion problems.

Earlier, Schulman[94] devised a two-compartment cell in which the separated aqueous phases were independently stirred from below while the "connecting" oil phase was stirred from above (see Figure 6). This apparatus has the advantage that the interface area remains constant, and therefore partition studies can be made on various solutes in the presence of trace amounts of surfactants (*e.g.*, phospholipids) at the oil–water interface.

Either type of apparatus is capable of providing useful information on the rate of transfer from one aqueous environment through an organic phase (simulating a membrane) to a second aqueous environment. If the solute is placed initially in compartment A at pH 2 and compartment C is at pH 7.4, one has a model for transport across the gastric membrane.

The basic importance of partitioning rate studies cannot be seriously questioned, but the interpretation of the results is still subject to some ambiguity. For example, Augustine and Swarbrick[158] used a Schulman-type cell to study the effect of lipid polarity on the rate of transport of salicylic acid. As the polarity of the lipid phase was increased (by increasing the mole fraction of isoamyl alcohol in cyclohexane), there was an increase in rate at which salicylic acid left the first aqueous phase. This is the expected result and confirms the work of Khalil and Martin[121] who used a Y-tube apparatus. However, this same increase in polarity also increased k_2, the rate at which salicylic acid left the lipid phase for the second aqueous phase. This is unexpected and contrary to Khalil and Martin's findings. Augustine and Swarbrick then found that, while keeping the surface to volume ratio constant, they could reverse the order of k_2 if they increased the stirring rate in the aqueous compartments. Then k_2 did decrease with increasing lipid polarity, and the value for k_1 was essentially unchanged.

Other discrepancies between measurements using the Y-tube and the Schulman cells have been noted, and it appears that some of the conditions assumed in the theoretical development that are not being met under all experimental conditions. For instance, it is assumed that the rate-determining step is the actual crossing of the interface boundary. This should be the case if the diffusion layer is of the order of magnitude of 30 μ in thickness.[94] Some care is required to adjust the stirring rate between that which is so slow that *diffusion* becomes rate determining and a stirring rate which is so great that nonlaminar flow breaks up the interface.

E. LIQUID ION-EXCHANGE MEDIA AND ION-SELECTIVE ELECTRODES

The application of partition coefficients to the study of liquid ion-selective electrodes has been discussed in section II.D. It should be emphasized that the selectivity is dependent upon the nature of the organic *solvent* and not on the nature of the site species (alkyl acid or amine).

F. MEASUREMENT OF HYDROPHOBIC BONDING ABILITY. STRUCTURE–ACTIVITY PARAMETERS

In the introduction it was pointed out that in the past decade far more partition coefficients have been determined in connection with biological structure–activity relationship studies than for all other purposes combined. A large number of these studies have already been referred to,[8,159] and the usefulness of the octanol–water parameter to predict the binding of solutes to serum albumin and to purified enzymes has been convincingly established.

(157) J. Doluisio and J. Swintosky, *J. Pharm. Sci.*, **53**, 597 (1964).

(158) M. Augustine and J. Swarbrick, *ibid.*, **59**, 314 (1970).

(159) W. Scholtan, K. Schlossman, and H. Rosenkranz, *Arzneim.-Forsch.*, **18**, 767 (1968).

Table XV

Improved π Values[a]

Function	*Phenoxyacetic acids*	*Function*	*Phenylacetic acids*	*Function*	*Benzoic acids*
3-F	0.22	3-Me	0.54	4-Cl	0.78
2-Cl	0.76	3-CF_3	1.21	3-OCH_2CO_2H	−0.76
2-Br	0.84	3-CN	−0.23		*Phenols*
4-Br	1.19	3-OCH_3	0.09	3-CN	0.22
4-I	1.43	3-CO_2H	−0.27	4-NH_2	−1.44
2-Me	0.84	3-SO_2CH_3	−1.35		*Anilines*
4-Me	0.60			4-OH	−0.86
2-Et	1.39				*Nitrobenzenes*
2-NO_2	−0.04			4-OCH_2CO_2H	−0.37

[a] Differing by more than 0.05 from those listed in ref 10.

Evidence is rapidly accumulating which supports the postulate that simple, nonspecific bonding of solutes is capable not only of markedly affecting enzyme action through allosteric effects, but that it often produces biologically important modifications of membrane function by a similar mechanism. For example, it has been shown that the action of alkanols in the protection of red cells against hypotonic hemolysis is a linear function of their hydrophobic character as measured by partitioning experiments[160] and, furthermore, that the concentration which affords hemolytic protection is very nearly the same as that which causes anesthesia.[161] The partition coefficient of alcohols between red cell ghosts and water has been measured, and it was found that in going from water to membrane, the free energy of transfer per methylene group was the same as that between water and octanol, namely, $\cong -690$ cal/mol.[161]

The usefulness of a "bonding" parameter based on partition values from a single reference system can be greatly extended if not every value required in every structure–activity study need be measured. The principles of additivity for the octanol–water system were covered in section V, and examples of how values in Table XVII can be systematically applied in this fashion are given in the following section.

VII. The Use of Table XVII

The amount of partitioning data uncovered in the present study was great enough to warrant its storage, manipulation, and retrieval by computer. It will be noted that some of the log $P_{octanol}$ values listed in Table XVII differ slightly from those published earlier from this laboratory. Generally, the differences resulted from the use of improved analytical techniques and the values in Table XVII should be considered more reliable. The significant changes in π constants from those contained in ref 10 appear in Table XV.

In Table XVII the data have been sorted in their most useful form; namely, the solutes are sorted first by empirical formula, then alphabetically by name, and finally by solvent syssystem.[162]

(160) H. Schneider, *Biochim. Biophys. Acta*, **163**, 451 (1968).

(161) P. Seeman, S. Roth, and H. Schneider, *ibid.*, **225**, 171 (1971).

(162) As stored in the computer, each solute has also been given a unique Wiswesser line notation ("The Wiswesser Line-Formula Chemical Notation," E. G. Smith, Ed., McGraw-Hill, New York, N. Y., 1968). A comparison of π values by functional groups is greatly facilitated by referring to a printout sorted by a permuted alphabetic listing by WLN notation.

The solute name appears in the right-hand column of Table XVII, and the reference from which the data were obtained appears in column 4. Column 6 lists the measured log *P* for the solute in the solvent system which appears in column 3. This value has been corrected for ionization, if any, and dimerization if measurements were reported over a sufficiently wide concentration range. The values are footnoted (column 5) as required. Column 7 lists the *calculated* log *P* for that solute in the octanol–water system. The regression equations used for this calculation appear in Table VIII together with the values for the standard deviation (*s*), the correlation coefficient (*r*), and the number of data points (*n*) which were available to establish the relationship. While the standard deviations indicate that some of these "regression values" are not sufficiently reliable for some purposes, nevertheless, they are useful in providing the only common scale of lipophilicity since only 20% of the values in the entire table are from a single system.

Space limitations and the absence of small letters and italics in computer printing precluded the use of the *Chemical Abstracts* system of nomenclature. For convenience in computer alphabetizing, the following rules were followed.

1. Aliphatic chains—branching: I = iso, S = secondary, and T = tertiary, as usual. "Normal" isomers are assumed if not specified; *i.e.*, BUTYRIC ACID = *n*-butanoic acid. N = nitrogen; *e.g.*, N-methylaniline.
2. Aliphatic chains—location from primary functional group is designated by Greek letter: A = α, B = β, G = γ, D = δ, E = ε, and W = ω; *e.g.*, A-BROMOPROPIONIC ACID.
3. Position on benzene rings
   (a) if only two functional groups or substituents: O = ortho, M = meta, and P = para, and the letter precedes the name; *e.g.*, O-NITROPHENOL.
   (b) if three or more substituents, numbering is from primary functional group; *e.g.*, 3,4-DIMETHYLPHENOL.
4. In all other ring systems, a numbering system is used regardless of the number of substituents; *e.g.*, 3-AMINOPYRIDINE, 2-NAPHTHOL.
5. For sorting and retrieval purposes, many trivial names were relegated to a secondary position; *e.g.*, M-DIHYDROXYBENZENE/RESORCINOL/; O-DIHYDROXYBENZENE/CATECHOL/.

6. In the empirical formula, the subscript 1 is expressed and not assumed.

It is unlikely that, for the foreseeable future, there will be measured log P values for more than a small fraction of the interesting molecules which might be needed in structure-activity work. One of the aims of this present article is to make it possible to calculate, with a reasonable degree of confidence, the log P values in one common system (octanol-water) for a wide variety of molecules for which values have not, or perhaps cannot, be determined. The present section will explain how the calculation procedures given in section V can be combined with the regression equations of Table VIII and the data in Table XVII to yield calculated values of the highest possible confidence level.

It was evident in section V that there are often several "routes" by which one can calculate a P_{octanol} value, depending upon the choice of "parent" molecule and how substructures are pieced together. If the computed values by all the "routes" agree within ± 0.1 log unit and also agree with any log P_{octanol} for that solute appearing in Table XVII as calculated from another solvent system, then one can accept an average value with some confidence. If there are some widely divergent values, however, then one must choose the "route" which has the greatest likelihood of yielding an accurate value. In order to help make such a choice, we have assigned "uncertainty units" (uu) to each type of calculation step so that the route with the lowest sum is the one which can be used with greatest confidence. Although these "u" units have been assigned by considering the average deviation in log P values of solutes with the required structural differences, and even though they can be directly added to the standard deviations of the regression equation values (see Table VIII), they are *not* to be considered as standard deviations in the strict sense. They are listed in Table XVI. The standard deviations of the observed log P_{octanol} values are used if given in the reference; otherwise, an arbitrary uu of 0.05 is taken.

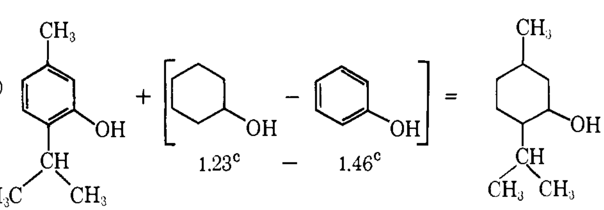
The following examples illustrate this procedure [the superscripts mean that the values were obtained from (a) Table VIII, standard deviation; (b) Table XVI; (c) Table XVII].

(A) Menthol: no log P_{oct} measured

(1) Regression from oil-water system

$$\log P_{\text{oct}} = (3.25^{c} \text{ and } 3.37^{c}) = \text{av } 3.31$$

$$uu = 0.28^{a}$$

(2) 

$$\log P_{\text{oct}} = 3.30^{c} + (-0.23) = 3.07$$

$$uu = 0.02^{b} + 0.04^{b} = 0.06$$

(3) $C_6H_5OH + (CH_3)_2CH- + -CH_3$

1.23 (1.50 − 0.20) 0.52

$$\log P_{\text{oct}} = 1.23^{c} + 1.30^{b} + 0.50^{b} = 3.03$$

Table XVI

"Uncertainty Units"

Calculation step or group	*π per step or group*	*Uncertainty units (uu)*	*Comments and exceptions*
1. $-CH_2-$	0.50	0.02	(a) π lower if between two very polar groups, *e.g.*, malonic acid (b) π lower if folding interaction possible (section V.D)
2. Branching			
(a) in C chain	−0.20	0.02	(a) Sign of π changes if steric blocking of polar group possible
(b) of functional group	−0.20	0.05	
(c) ring closure	−0.09	0.02	
3. Double bond	−0.30	0.03	
4. Folding	−0.60	0.05	(a) See unusual case of phenoxyacetamides (section V.D)
5. Intramolecular H-bonding	0.65	0.10	
6. Equivalence of aliphatic OH and NH_2	0.00	0.05	
7. Aliphatic groups			
(a) -COOH	−0.65	0.03	
(b) -OH	−1.16	0.03	
(c) $-NH_2$	−1.16	0.03	
(d) -C=O	−1.21	0.03	
(e) -CN	−0.84	0.04	
(f) -O-	−0.98	0.05	
(g) $-CONH_2$	−1.71	0.05	
(h) -F	−0.17	0.03	
(i) -Cl	0.39	0.04	
(j) -Br	0.60	0.04	
(k) -I	1.00	0.05	

For aromatic substituents, use π values and standard deviations (as uu) appearing in T. Fujita, *et al.*, *J. Am. Chem. Soc.*, **86,** 5175 (1964).

$$uu = 0.02^{b} + 0.08^{b} + 0.02^{b} = 0.12$$

Route 2 should be chosen for several reasons. It has the lowest uu value. The electronic effect on π of the difference between an aliphatic and aromatic OH group is precisely allowed for. Adding the isopropyl group adjacent to the OH in route 3 may involve a steric blocking of its hydrophilic character.

(B) *n*-Propylamine: no log P_{oct} measured

(1) Equivalence of OH and NH_2

$$\log P_{\text{oct}} \text{ (propanol)} = 0.34^{c}$$

$$uu = 0.07^{b}$$

(2) $(CH_3CHNH_2CH_3)$ − (branch)

$$\log P_{\text{oct}} = -0.03^{c} - (-0.20)^{b} = 0.17$$

$$uu = 0.02^{b} + 0.05^{b} = 0.07$$

(3) *n*-Propylamine

$\log P_{oct}$ (regression from ether–water) = 0.37

uu = 0.27[a]

(4) *n*-Butylamine − methyl

$\log P_{oct} = 0.81^c - 0.50^b = 0.31$

$uu = 0.02^b + 0.02^b = 0.04$

Since route 4 has the lowest uu and is reinforced by (1) and (3), it is preferred over (2).

(C) Lactic acid: $\log P_{oct} = -0.62^c$

(1) Hydroxyacetic acid + methyl + branch = $CH_3CHOHCO_2H$

$\log P_{oct} = -1.11^c + 0.50^b + (-0.20)^b = -0.81$

$uu = 0.05^c + 0.02^b + 0.05^b = 0.12$

(2) Regression from ether–water

$\log P_{oct}$ (av of 5) = −0.80

uu = 0.19[a]

(3) $(CH_3)_2C(OH)CO_2H$ − methyl − branch = lactic acid

$\log P_{oct} = -0.36^c - 0.50^b - (-0.20)^b = -0.68$

$uu = 0.05^c + 0.02^b + 0.02^b = 0.09$

The measured $\log P_{oct}$ agrees quite well with that arrived at by route 3. The values arrived at by routes 1 and 2 should not be totally disregarded, however, because the presence of an appreciable amount of polylactic acid impurity in the sample measured by Collander could be responsible for an observed value which was 0.1 to 0.2 unit too high.

(D) Acetonylacetone: $\log P_{oct}$ not measured

	log *P*	uu
(1) Regression from ether–water	−0.19	0.19[a]
(2) Log P_{oct} (acetone)[c] × 2	−0.48	0.10

(3) 2-Butanone + acetone − methyl = $CH_3COCH_2CH_2COCH_3$

$\log P_{oct} = 0.29^c + (-0.24)^c - 0.50^b = -0.45$

$uu = 0.02^c + 0.05^c + 0.02^b = 0.09$

The choice clearly favors the range −0.45 to −0.48.

(E) Levulinic acid: $\log P_{oct}$ not measured

(1) $CH_3COCH_3 + CH_3CO_2H = CH_3COCH_2CH_2CO_2H$

$\log P_{oct} = -0.24^c + (-0.17)^c = -0.41$

$uu = 0.05^c + 0.02^c = 0.07$

(2) 2-Butanone + aliphatic $-CO_2H$

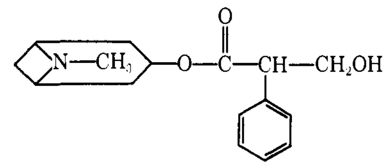
$\log P_{oct} = 0.29^c + (-0.65)^b = -0.36$

$uu = 0.02^c + 0.03^b = 0.05$

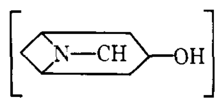
	log *P*	uu
(3) Regression from ether–water (av 3)	−0.40	0.19[a]
(4) Regression from *i*-BuOH–water	−0.39	0.14[a]
(5) Regression from $CHCl_3$–water (av 2)	0.08	0.27[a]

Clearly the value by route 5 is eliminated from consideration and a value in the range of −0.36 to −0.40 is preferred.

(F) Atropine



(1)



− [OH] + [$C_6H_5CH_2CO_2H$] + [CH_2OH] + [branch]

$\log P_{oct} = -0.28^c - (-1.16)^b + 1.30^c + (-0.66)^c + -0.20^b = 1.32$

$uu = 0.27^a + 0.05^b + 0.02^c + 0.02^c + 0.02^c = 0.38$

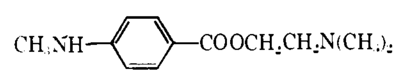
(2) As (1) but log *P* tropine regr. from *i*-BuOH–water

$\log P_{i\text{-BuOH}} = 0.21^c - (-1.16)^b + 1.30^c + (-0.66)^c + (-0.20)^b = 1.81$

$uu = 0.15^a + 0.05^b + 0.02^c + 0.02^c + 0.02^c = 0.26$

The measured $\log P_{oct}$ for atropine is 1.81 which is in agreement with route 2. The uncertainty of route 1 is not that much worse than (2), but the measured value for tropine in ether–water appears very doubtful.

(G) *p*-*N*-Methylaminobenzoic acid, *N*,*N*-dimethylaminoethyl ester



(1) $CH_3NH- + (C_6H_5COOCH_2-) + (-CH_2N(CH_3)_2)$

$\log P = (0.50^b - 1.23^*) + 2.12^c + 0.27^c = (1.66)$

$uu = 0.01^b + 0.02^b + 0.02^b + 0.05^d = (0.10)$

$\log P_{(corr)}$[163] = 2.03

uu = 0.18

(2) Regression from oil–water

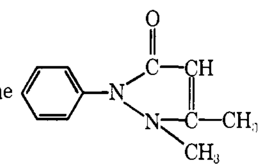
$\log P_{oct} = 2.01^c$

uu = 0.29[a]

(3) Log P_{oct} (measured) = 1.95[c]

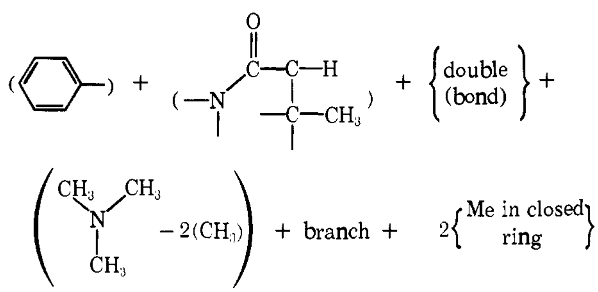
In these first examples, the amount of interaction between the component parts used in the calculations was either small or it could be taken into consideration (as in G). In the following example this is not the case, and it can be seen that it is possible to use the proposed method of calculation to support an erroneous measured value.

(163) $\pi_{NH_2} = -1.23$ uses benzene as the "parent." Correcting for electronic effects (ref 10) using σ ($-COCH_3$) = 0.39, we correct π by 0.37 and add to the uu by 0.08.

(H) Antipyrene 

	log P	uu
(1) Log P_{oct} regression from ether–water	-0.06^{c}	0.27^{a}
(2) Log P_{oct} regression from $CHCl_3$–water	0.53^{c}	0.27^{a}
(3) Log P_{oct} regression from oil–water	-0.12^{c}	0.28^{a}
	0.15^{c}	0.28^{a}
(4) Log P_{oct} regression from i-BuOH–water	0.21^{c}	0.15^{a}

The value of 0.21 should be favored because it has the lowest uu value, but one could attempt to verify it by calculation.

(5) 

$$\text{Log } P = 2.13^{c} + (-0.21)^{c} + (-0.30)^{b} + (0.27^{c} - 1.0)^{b} + (-0.20)^{b} + (-0.18)^{b} = 0.53$$

$$\text{uu} = 0.02^{c} + 0.02^{c} + 0.03^{b} + 0.05^{c} + 0.04^{b} + 0.02^{b} + 0.04^{b} = 0.22$$

Without any allowance for an interaction between the amide and amine nitrogen atoms, route 5 would support route 2. With such a variety of values to choose from and no clear preference indicated by uu values, the only safe course is to measure the P value directly. In this case log P_{oct} turned out to be 0.23 and the route 4 was vindicated.

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VIII. Glossary of Terms

A^-	anionic form of acidic solute
α	degree of ionization
B	neutral form of basic solute
BH^+	protonated form of basic solute
C	molar concentration
cmc	critical micelle concentration (molar)
E_s	steric parameter as defined by Taft
$\langle\epsilon\rangle_j$	average energy level of jth group
G	free energy
H	enthalpy
HA	neutral form of acidic solute
H_2C	dihydric complexing agent
HLB	hydrophile–lipophile balance
K_A	dissociation constant of single molecules into ions in aqueous phase
K_{assoc}	association constant of single into double molecules in lipoid phase; equals $1/K_D$
K_D	dissociation constant of double into single molecules in lipoid phase
K_{HB}	association constant between hydrogen bond donor and acceptor
K_f	association constant for formation of complex or imine
k	Boltzman constant
L	milliliters of lipoid extracting phase
M^{n+}	metal ion carrying charge of n^+
N	(in counter-current distribution) position of peak
N	(in partition calculation) concentration of un-ionized solute in water at first concentration level (in mol/l.)
n	(in counter-current distribution) total number of tubes
n	(in partition calculation) concentration of un-ionized solute at second concentration level (in mol/l.)
n	(in regression equations) number of data points treated
(o)	organic (or oil) phase
P	partition coefficient; nonpolar/polar phase; refers to concentration of neutral solute unless specified (only exception is in eq 19 and 20 where P refers to pressure)
P^*	apparent partition coefficient (total solute measured, regardless of form)
P'	thermodynamic partition coefficient = ratio of mole fractions in nonpolar/polar phases.
pK_a	negative logarithm of acid ionization constant
π	hydrophobic substituent constant; $\pi_X = \log P_X - \log P_H$
R	gas constant
r	(in regression equations) correlation coefficient
r	(in counter-current distribution) specific tube number
s	standard deviation
S	entropy
σ	electronic parameter as defined by Hammett
T	(in counter-current distribution) fraction of total solute
T	absolute temperature
μ	chemical potential (per mole)
$\bar{V}_s$	molar volume of solvent
W	ml of aqueous solution being extracted
(w)	water phase
X	mole fraction
Z	particle partition function (quantum mechanics)
ψ	state function (quantum mechanics)

Table XVII. SORTED BY EMPIRICAL FORMULA, THEN NAME, THEN SOLVENT NUMBER, THEN REFERENCE. MEASURED "LOGP OCT" FOLLOWED BY "*"; OTHERS CALC FROM SPECIFIED EQ IN TABLE VIII

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1	OILS	164	22	0.60	0.94 B	AR1	ARGON
2	NITROBENZENE	92	46	-5.04		BR1K1	POTASSIUM BROMIDE
3	CCL4	165		1.35		BR2	BROMINE
4	CS2	165		1.89		BR2	BROMINE
5	BROMOFORM	166		1.80		BR2	BROMINE
6	N-BUTANOL	91	46	-1.82	-3.03	CL1CS1	CESIUM CHLORIDE
7	N-BUTANOL	91	46	-1.74	-2.92	CL1K1	POTASSIUM CHLORIDE
8	N-BUTANOL	94	46	-1.74	-2.94	CL1K1	POTASSIUM CHLORIDE
9	NITROBENZENE	92	46	-5.36		CL1K1	POTASSIUM CHLORIDE
10	N-BUTANOL	91	46	-1.55	-2.66	CL1LI1	LITHIUM CHLORIDE
11	N-BUTANOL	91	46	-1.76	-2.96	CL1NA1	SODIUM CHLORIDE
12	N-BUTANOL	94	46	-1.74	-2.94	CL1NA1	SODIUM CHLORIDE
13	SEC-BUTANOL	94	46	-1.19		CL1NA1	SODIUM CHLORIDE
14	N-BUTANOL	91	46	-1.74	-2.92	CL1RB1	RUBIDIUM CHLORIDE
15	CCL4	167	51	1.29		CL2	CHLORINE
16	OILS	168	46	-0.46	0.06 B	CL2HG1	MERCURIC CHLORIDE
17	DIETHYL ETHER	2		-1.74	-1.42 A	D2O1	DEUTERIUM OXIDE
18	OILS	2		-3.15	-1.64 A	D2O1	DEUTERIUM OXIDE
19	OILS	164	22	0.23	0.66 B	HE1	HELIUM
20	CCL4	169		0.54		I1BR1	IODINE MONOBROMIDE
21	CCL4	169		-0.70		I1CL1	IODINE MONOCHLORIDE
22	NITROBENZENE	92	46	-3.74		I1K1	POTASSIUM IODIDE
23	NITROBENZENE	92	46	-5.00		I1LI1	LITHIUM IODIDE
24	NITROBENZENE	92	46	-4.59		I1NA1	SODIUM IODIDE
25	NITROBENZENE	92	46	-3.60		I1RB1	RUBIDIUM IODIDE
26	CHCL3	165		2.12		I2	IODINE
27	BENZENE	170		2.59		I2	IODINE
28	NITROBENZENE	170		2.29		I2	IODINE
29	PRIM. PENTANOLS	47		-1.66		I2	IODINE
30	CCL4	166		1.93		I2	IODINE
31	CS2	166		2.77		I2	IODINE
32	DODECANE	165		1.87		I2	IODINE
33	HEXADECANE	165		1.59		I2	IODINE
34	BROMOFORM	166		2.62		I2	IODINE
35	OILS	164	22	0.88	1.16 B	KR1	KRYPTON
36	OILS	164	22	0.55	0.92 B	N2	NITROGEN
37	CCL4	171		1.15		O4OS1	OSMIUM TETROXIDE
38	CCL4	172		1.09		O4OS1	OSMIUM TETROXIDE
39	OILS	164	22	2.04	2.05 B	RO1	RADON
40	OILS	164	22	1.16	1.37 B	XE1	XENON
41	OILS	173		-1.04	0.25 A	H1CL1	HYDROGEN CHLORIDE
42	DIETHYL ETHER	174		-0.64	-0.44 A	H1F1	HYDROFLUDRIC ACID
43	CHCL3	174	12	-2.92	-1.43 A	H1F1	HYDROFLUORIC ACID
44	DIETHYL ETHER	175	26	0.84	0.86 A	H1N3	HYDROGEN AZIDE
45	DIETHYL ETHER	174		0.86	0.88 A	H1N3	HYDROGEN AZIDE
46	CHCL3	174		-0.16	1.07 A	H1N3	HYDROGEN AZIDE
47	SEC-BUTANOL	84		-0.44	-1.15	H2O1	WATER
48	DIETHYL ETHER	176		-1.18	-0.92 A	H2O2	HYDROGEN PEROXIDE
49	DIETHYL ETHER	177		-1.36	-1.08 A	H2O2	HYDROGEN PEROXIDE
50	DIETHYL ETHER	178		-0.94	-0.70	H2O2	HYDROGEN PEROXIDE
51	DIETHYL ETHER	174		-1.19	-0.92 A	H2O2	HYDROGEN PEROXIDE
52	CHCL3	179	26	-2.78	-1.29 A	H2O2	HYDROGEN PEROXIDE
53	CHCL3	174	12	-3.34	-1.82 A	H2O2	HYDROGEN PEROXIDE
54	BENZENE	179	26	-2.30	-0.89 A	H2O2	HYDROGEN PEROXIDE
55	1-BUTANOL	179	26	-0.48	-1.19	H2O2	HYDROGEN PEROXIDE
56	I-BUTANOL	178		-0.41	-1.09	H2O2	HYDROGEN PEROXIDE
57	NITROBENZENE	179	26	-2.30	-1.03	H2O2	HYDROGEN PEROXIDE
58	PRIM. PENTANOLS	177		-0.85	-1.38	H2O2	HYDROGEN PEROXIDE
59	PRIM. PENTANOLS	180		-0.85	-1.37	H2O2	HYDROGEN PEROXIDE
60	ETHYL ACETATE	178		-0.60	-0.70	H2O2	HYDROGEN PEROXIDE
61	1-PENT. ACETATE	178		-1.11	-1.33	H2O2	HYDROGEN PEROXIDE
62	N-BUTANOL	181	10	-1.00		H2O4P1	ORTHOPHOSPHATE ANION
63	HEXANOL	181	18	-0.52		H2O4P1	ORTHOPHOSPHATE ANION
64	N-BUTANOL	181	10	0.30		H2O7P2	PYROPHOSPHATE ANION
65	HEXANOL	181	18	0.73		H2O7P2	PYROPHOSPHATE ANION
66	DIETHYL ETHER	174		0.95	0.96 A	H2S1	HYDROGEN SULFIDE
67	CHCL3	174		0.89	1.44 N	H2S1	HYDROGEN SULFIDE
68	DIETHYL ETHER	174		-1.96	-0.90 B	H3N1	AMMONIA
69	CHCL3	174		-1.35	-1.37 B	H3N1	AMMONIA
70	SEC-BUTANOL	84	19	-1.09	-2.04	H3N1	AMMONIA
71	TOLUENE	68		-1.40	-0.35 B	H3N1	AMMONIA
72	PRIM. PENTANOLS	182		-0.85	-1.49	H3N1	AMMONIA
73	CCL4	7		-2.35	-1.56 B	H3N1	AMMONIA
74	DIETHYL ETHER	174		-2.28	-1.87 A	H3N1O1	HYDROXYLAMINE
75	CHCL3	174		-2.58	-1.13 A	H3N1O1	HYDROXYLAMINE
76	DIETHYL ETHER	174		-2.34	-1.23 B	H4N2	HYDRAZINE
77	CHCL3	174		-1.35	-1.37 B	H4N2	HYDRAZINE
78	BENZENE	183		-1.65	-0.60 B	H4N2	HYDRAZINE
79	1-BUTANOL	184		-0.66		H5N1O1	AMMONIUM HYDROXIDE
80	PRIM. PENTANOLS	184		-0.87		H5N1O1	AMMONIUM HYDROXIDE
81	OILS	173		0.20	0.64 B	C1CL1N1	CYANOGEN CHLORIDE
82	OILS	173		2.42	2.44 B	C1CL3N1O2	CHLOROPICRIN
83	OILS	173		2.66	2.64 B	C1CL4	CARBON TETRACHLORIDE
84	CCL4	185		-0.75		C1I1N1	IODINE CYANIDE
85	OILS	173		2.08	2.16 B	C1S2	CARBON DISULFIDE
86	OILS	82		1.70	1.84 B	C1S2	CARBON DISULFIDE
87	OCTANOL	186		1.97	1.97 *	C1H1CL3	CHLOROFORM
88	OILS	173		1.86	1.98 B	C1H1CL3	CHLOROFORM
89	DIETHYL ETHER	187		0.38	0.45 A	C1H1N1	HYDROCYANIC ACID
90	DIETHYL ETHER	174		0.26	0.35 A	C1H1N1	HYDROCYANIC ACID
91	CHCL3	187		-0.67		C1H1N1	HYDROCYANIC ACID
92	CHCL3	174		-0.66	0.62 A	C1H1N1	HYDROCYANIC ACID
93	BENZENE	187		-0.35	1.07 A	C1H1N1	HYDROCYANIC ACID
94	BENZENE	188	12	-0.57	0.81 A	C1H1N1	HYDROCYANIC ACID
95	CCL4	187		-1.38		C1H1N1	HYDROCYANIC ACID
96	ETHYL BROMIDE	187		-0.45		C1H1N1	HYDROCYANIC ACID
97	BROMOETHANE	187		-0.45		C1H1N1	HYDROCYANIC ACID
98	DIETHYL ETHER	3		-0.96	-0.72 A	C1H2N2	CYANAMIDE
99	OILS	2		-2.35	-0.91 A	C1H2N2	CYANAMIDE
100	PRIM. PENTANOLS	189		-0.30	-0.68	C1H2N2	CYANAMIDE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
101	ETHYL ACETATE	189	12	-0.19	-0.26	C1H2N2	CYANAMIDE
102	DI-I-PR. ETHER	189	12	-0.71	-0.28	C1H2N2	CYANAMIDE
103	ME-I-BUT.KETONE	189		-0.23	-0.27	C1H2N2	CYANAMIDE
104	DIETHYL ETHER	188	12	-0.96	0.00 B	C1H2O1	FORMALDEHYDE
105	OCTANOL	5		-0.54	-0.54 =	C1H2O2	FORMIC ACID
106	DIETHYL ETHER	190		-0.52	-0.34 A	C1H2O2	FORMIC ACID
107	DIETHYL ETHER	191		-0.40	-0.31 A	C1H2O2	FORMIC ACID
108	DIETHYL ETHER	192		-0.45	-0.28 A	C1H2O2	FORMIC ACID
109	DIETHYL ETHER	46		-0.40	-0.23 A	C1H2O2	FORMIC ACID
110	DIETHYL ETHER	36		-0.43	-0.25 A	C1H2O2	FORMIC ACID
111	CHCL3	45	12	-2.50	-1.03 A	C1H2O2	FORMIC ACID
112	CHCL3	36		-2.12	-0.69 A	C1H2O2	FORMIC ACID
113	OILS	193		-1.84	-0.44 A	C1H2O2	FORMIC ACID
114	BENZENE	45		-2.95	-1.55 A	C1H2O2	FORMIC ACID
115	BENZENE	44		-2.70	-1.28 A	C1H2O2	FORMIC ACID
116	BENZENE	193		-2.57	-1.15 A	C1H2O2	FORMIC ACID
117	N-BUTANOL	190		-0.08	-0.62	C1H2O2	FORMIC ACID
118	SEC-BUTANOL	190		0.03	-0.47	C1H2O2	FORMIC ACID
119	XYLENE	193		-2.38	-0.97 A	C1H2O2	FORMIC ACID
120	TOLUENE	193		-2.58		C1H2O2	FORMIC ACID
121	TOLUENE	41		-2.66	-0.73 A	C1H2O2	FORMIC ACID
122	NITROBENZENE	48		-1.67	-0.51	C1H2O2	FORMIC ACID
123	PRIM. PENTANOLS	190		-0.26	-0.73	C1H2O2	FORMIC ACID
124	ETHYL ACETATE	194		-0.23	-0.30	C1H2O2	FORMIC ACID
125	CCL4	45	26	-3.12		C1H2O2	FORMIC ACID
126	DI-I-PR. ETHER	190		-0.84	-0.42	C1H2O2	FORMIC ACID
127	2-BUTANONE	190		0.12	0.39	C1H2O2	FORMIC ACID
128	ME-I-BUT.KETONE	195		-0.34	-0.37	C1H2O2	FORMIC ACID
129	ME-I-BUT.KETONE	196		-0.38	-0.40	C1H2O2	FORMIC ACID
130	OLEYL ALCOHOL	5		-0.92	-0.35	C1H2O2	FORMIC ACID
131	O-NITROTOLUENE	48		-1.81		C1H2O2	FORMIC ACID
132	S-PENTANOLS	190	12	0.07	-0.22	C1H2O2	FORMIC ACID
133	S-PENTANOLS	195		-0.22	-0.56	C1H2O2	FORMIC ACID
134	CS2	193		-3.23		C1H2O2	FORMIC ACID
135	PARAFFINS	197		-2.90		C1H2O2	FORMIC ACID
136	OCTANOL	5		1.69	1.69 =	C1H3I1	METHYL IODIDE
137	DIETHYL ETHER	3		1.92	1.80 A	C1H3I1	METHYL IODIDE
138	DIETHYL ETHER	3		-2.85	-1.67 B	C1H3N1O1	FORMAMIDE
139	OILS	2		-3.12	-1.61 A	C1H3N1O1	FORMAMIDE
140	OCTANOL	186		-0.33	-0.33 =	C1H3N1O2	NITROMETHANE
141	OCTANOL	5		0.08	0.08 =	C1H3N1O2	NITROMETHANE
142	CYCLOHEXANE	141		-0.93		C1H3N1O2	NITROMETHANE
143	OILS	173		-0.32	0.17 B	C1H3N1O2	NITROMETHANE
144	DIETHYL ETHER	3		-3.33	-2.79 A	C1H4N2O1	UREA
145	DIETHYL ETHER	112		-3.52	-2.96 A	C1H4N2O1	UREA
146	DIETHYL ETHER	198		-3.30	-2.76 A	C1H4N2O1	UREA
147	CHCL3	112		-3.85	-2.97 N	C1H4N2O1	UREA
148	OILS	2		-3.82	-2.26 A	C1H4N2O1	UREA
149	OCTANOL	9		-1.14	-1.14 =	C1H4N2S1	THIOUREA
150	DIETHYL ETHER	3		-2.20	-1.80 A	C1H4N2S1	THIOUREA
151	DIETHYL ETHER	112		-2.10	-1.70 A	C1H4N2S1	THIOUREA
152	DIETHYL ETHER	198		-2.14	-0.95 A	C1H4N2S1	THIOUREA
153	CHCL3	112	12	-3.10	-2.38 N	C1H4N2S1	THIOUREA
154	OILS	2		-2.92	-1.43 A	C1H4N2S1	THIOUREA
155	OCTANOL	186		-0.66	-0.66 =	C1H4O1	METHANOL
156	OCTANOL	5		-0.82	-0.82 =	C1H4O1	METHANOL
157	DIETHYL ETHER	3		-0.85	-0.63 A	C1H4O1	METHANOL
158	DIETHYL ETHER	174		-1.29	-1.00 A	C1H4O1	METHANOL
159	CYCLOHEXANE	199		-1.84		C1H4O1	METHANOL
160	CHCL3	174		-1.36	-0.66 N	C1H4O1	METHANOL
161	OILS	173		-1.96	-0.55 A	C1H4O1	METHANOL
162	OILS	101		-2.01	-0.63 A	C1H4O1	METHANOL
163	OILS	200		-2.11	-0.73 A	C1H4O1	METHANOL
164	OILS	201		-2.02	-0.65 A	C1H4O1	METHANOL
165	NITROBENZENE	202		-1.60	-0.46	C1H4O1	METHANOL
166	OCTANOL	5		-0.57	-0.57 =	C1H5N1	METHYLAMINE
167	DIETHYL ETHER	3		-1.64	-0.60 B	C1H5N1	METHYLAMINE
168	CHCL3	203	12	-0.56	-0.71 B	C1H5N1	METHYLAMINE
169	CHCL3	68		-0.90	-1.00 B	C1H5N1	METHYLAMINE
170	CHCL3	204		-1.09	-1.15 B	C1H5N1	METHYLAMINE
171	BENZENE	205		-1.34	0.37 B	C1H5N1	METHYLAMINE
172	1-BUTANOL	184		0.00	-0.52	C1H5N1	METHYLAMINE
173	XYLENE	46		-1.00	-0.43 B	C1H5N1	METHYLAMINE
174	TOLUENE	205		-1.40	-0.35 B	C1H5N1	METHYLAMINE
175	PRIM. PENTANOLS	182		-0.45	-0.98	C1H5N1	METHYLAMINE
176	OCTANOL	206		2.44	2.44 =	C2H1BR2N3	1,2,3-TRIAZOLE,4,5-DIBROMO
177	OCTANOL	206		2.24	2.24 =	C2H1BR2N3	1,2,4-TRIAZOLE,3,5-DIBROMO
178	DIETHYL ETHER	3		1.57	1.49 A	C2H1CL3O2	TRICHLOROACETIC ACID
179	DIETHYL ETHER	207		1.21	1.18 A	C2H1CL3O2	TRICHLOROACETIC ACID
180	DIETHYL ETHER	113		1.63	1.54 A	C2H1CL3O2	TRICHLOROACETIC ACID
181	DIETHYL ETHER	46		1.78	1.68 A	C2H1CL3O2	TRICHLOROACETIC ACID
182	CHCL3	43		-0.69	0.61 A	C2H1CL3O2	TRICHLOROACETIC ACID
183	BENZENE	208		-1.30	0.10 A	C2H1CL3O2	TRICHLOROACETIC ACID
184	TOLUENE	43		-0.98	0.72 A	C2H1CL3O2	TRICHLOROACETIC ACID
185	NITROBENZENE	43		0.04	0.91	C2H1CL3O2	TRICHLOROACETIC ACID
186	PRIM. PENTANOLS	43		1.79	1.96	C2H1CL3O2	TRICHLOROACETIC ACID
187	BROMOETHANE	43		-0.26		C2H1CL3O2	TRICHLOROACETIC ACID
188	IODOMETHANE	41		-1.06		C2H1CL3O2	TRICHLOROACETIC ACID
189	DIETHYL ETHER	192		1.24	1.20 A	C2H2CL2O2	DICHLOROACETIC ACID
190	DIETHYL ETHER	113		1.46	1.39 A	C2H2CL2O2	DICHLOROACETIC ACID
191	DIETHYL ETHER	46		1.31	1.27 A	C2H2CL2O2	DICHLOROACETIC ACID
192	CHCL3	113		-0.89	0.41 A	C2H2CL2O2	DICHLOROACETIC ACID
193	OILS	209		-0.30	0.94 A	C2H2CL2O2	DICHLOROACETIC ACID
194	BENZENE	208		-1.40	0.00 A	C2H2CL2O2	DICHLOROACETIC ACID
195	TOLUENE	43		-1.42	0.33 A	C2H2CL2O2	DICHLOROACETIC ACID
196	NITROBENZENE	43		-0.10	0.79	C2H2CL2O2	DICHLOROACETIC ACID
197	CCL4	43	12	-2.31	-0.14 A	C2H2CL2O2	DICHLOROACETIC ACID
198	IODOMETHANE	41		-1.15		C2H2CL2O2	DICHLOROACETIC ACID
199	OCTANOL	56		1.04	1.04 =	C2H2CL3N1O1	TRICHLOROACETAMIDE
200	DIETHYL ETHER	113		1.08	1.06 A	C2H2CL3N1O1	TRICHLOROACETAMIDE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
201	CHCL3	113		0.31	0.87 N	C2H2CL3N1O1	TRICHLOROACETAMIDE
202	OCTANOL	210		0.12	0.12 =	C2H2F3N1O1	TRIFLUOROACETAMIDE
203	DIETHYL ETHER	211		-1.02	-0.78 A	C2H2O4	OXALIC ACID
204	DIETHYL ETHER	212		-0.94	-0.71 A	C2H2O4	OXALIC ACID
205	DIETHYL ETHER	3		-0.92	-0.69 A	C2H2O4	OXALIC ACID
206	DIETHYL ETHER	46		-0.72	-0.51 A	C2H2O4	OXALIC ACID
207	DIETHYL ETHER	213		-0.91	-0.67 A	C2H2O4	OXALIC ACID
208	DIETHYL ETHER	36		-0.87	-0.64 A	C2H2O4	OXALIC ACID
209	N-BUTANOL	194		-0.76	-0.53	C2H2O4	OXALIC ACID
210	PRIM. PENTANOLS	182		-0.30	-0.78	C2H2O4	OXALIC ACID
211	ETHYL ACETATE	194		-0.34	-0.43	C2H2O4	OXALIC ACID
212	HEXANOL	74		-0.48		C2H2O4	OXALIC ACID
213	ME-1-BUT.KETONE	195		-0.69	-0.64	C2H2O4	OXALIC ACID
214	S-PENTANOLS	195		-0.44	-0.81	C2H2O4	OXALIC ACID
215	OCTANOL	5		0.41	0.41 =	C2H3BR1O2	BROMOACETIC ACID
216	DIETHYL ETHER	192		0.64	0.68 A	C2H3BR1O2	BROMOACETIC ACID
217	CHCL3	46		-1.14	0.18 A	C2H3BR1O2	BROMOACETIC ACID
218	OILS	209		-0.72	0.56 A	C2H3BR1O2	BROMOACETIC ACID
219	BENZENE	29		-1.41	-0.01 A	C2H3BR1O2	BROMOACETIC ACID
220	XYLENE	46		-1.37	0.29 A	C2H3BR1O2	BROMOACETIC ACID
221	TOLUENE	29		-1.55	0.24 A	C2H3BR1O2	BROMOACETIC ACID
222	OILS	214		-0.18	1.06 A	C2H3BR3O2	2,2,2-TRIBROMO-1,1-ETHANEDIOL /BROMALHYDRATE/
223	DIETHYL ETHER	192		0.41	0.47 A	C2H3CL1O2	CHLOROACETIC ACID
224	DIETHYL ETHER	113		0.42	0.48 A	C2H3CL1O2	CHLOROACETIC ACID
225	DIETHYL ETHER	46		0.39	0.47 A	C2H3CL1O2	CHLOROACETIC ACID
226	DIETHYL ETHER	40		0.02	0.14 A	C2H3CL1O2	CHLOROACETIC ACID
227	DIETHYL ETHER	188		0.37	0.45 A	C2H3CL1O2	CHLOROACETIC ACID
228	CHCL3	43		-1.67	-0.28 A	C2H3CL1O2	CHLOROACETIC ACID
229	CHCL3	113		-1.35	-0.01 A	C2H3CL1O2	CHLOROACETIC ACID
230	CHCL3	46		-1.92	-0.53 A	C2H3CL1O2	CHLOROACETIC ACID
231	OILS	209		-1.10	0.24 A	C2H3CL1O2	CHLOROACETIC ACID
232	BENZENE	215		-1.45	-0.05 A	C2H3CL1O2	CHLOROACETIC ACID
233	BENZENE	42		-1.60	-0.19 A	C2H3CL1O2	CHLOROACETIC ACID
234	TOLUENE	43		-2.00	-0.17 A	C2H3CL1O2	CHLOROACETIC ACID
235	TOLUENE	40		-2.12	-0.28 A	C2H3CL1O2	CHLOROACETIC ACID
236	TOLUENE	42		-1.74	0.05 A	C2H3CL1O2	CHLOROACETIC ACID
237	TOLUENE	42		-1.74	0.06 A	C2H3CL1O2	CHLOROACETIC ACID
238	NITROBENZENE	43		-0.85	0.17	C2H3CL1O2	CHLOROACETIC ACID
239	NITROBENZENE	42	12	1.15	1.83 A	C2H3CL1O2	CHLOROACETIC ACID
240	CCL4	43		-2.56	-0.33 A	C2H3CL1O2	CHLOROACETIC ACID
241	IODOMETHANE	41		-1.36		C2H3CL1O2	CHLOROACETIC ACID
242	DIETHYL ETHER	3		0.63	0.67 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
243	DIETHYL ETHER	188		0.63	0.67 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
244	DIETHYL ETHER	174		0.60	0.65 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
245	CHCL3	174		-0.96	0.34 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
246	OILS	214		-0.66	0.62 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
247	OILS	70		-0.75	0.42 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
248	TOLUENE	188	12	-1.76	0.04 A	C2H3CL3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE/
249	DIETHYL ETHER	112		-0.27	-0.12 A	C2H3F1O2	FLUOROACETIC ACID
250	CHCL3	112		-1.96	-0.57 A	C2H3F1O2	FLUOROACETIC ACID
251	OCTANOL	9		0.41	0.41 =	C2H3F3O1	ETHANOL, 2,2,2-TRIFLUORO
252	OCTANOL	216		0.32	0.32 =	C2H3F3O1	2,2,2-TRIFLUOROETHANOL
253	DIETHYL ETHER	3		0.86	0.87 A	C2H3I1O2	IODOACETIC ACID
254	DIETHYL ETHER	112		0.83	0.84 A	C2H3I1O2	IODOACETIC ACID
255	CHCL3	112		-0.82	0.47 A	C2H3I1O2	IODOACETIC ACID
256	CHCL3	29		-0.79	0.50 A	C2H3I1O2	IODOACETIC ACID
257	OILS	209		-0.46	0.83 A	C2H3I1O2	IODOACETIC ACID
258	BENZENE	29		-1.08	0.31 A	C2H3I1O2	IODOACETIC ACID
259	TOLUENE	29		-1.22	0.50 A	C2H3I1O2	IODOACETIC ACID
260	OCTANOL	186		-0.34	-0.34 =	C2H3N1	ACETONITRILE
261	DIETHYL ETHER	3		-0.22	-0.08 A	C2H3N1	ACETONITRILE
262	DIETHYL ETHER	207		-1.49	-1.19 A	C2H3N1O3	OXAMIC ACID
263	OCTANOL	210		-0.52	-0.52 =	C2H4BR1N1O1	BROMOACETAMIDE
264	OCTANOL	56		-0.53	-0.53 =	C2H4CL1N1O1	CHLOROACETAMIDE
265	DIETHYL ETHER	3		-1.02	-0.78 A	C2H4CL1N1O1	CHLOROACETAMIDE
266	DIETHYL ETHER	113		-1.03	-0.79 A	C2H4CL1N1O1	CHLOROACETAMIDE
267	CHCL3	113		-0.96	-0.29 N	C2H4CL1N1O1	CHLOROACETAMIDE
268	OCTANOL	210		-1.05	-1.05 =	C2H4F1N1O1	FLUOROACETAMIDE
269	OCTANOL	210		-0.19	-0.19 =	C2H4I1N1O1	IODOACETAMIDE
270	DIETHYL ETHER	112		1.23	1.20 A	C2H4N2S2	OXAMIDE,DITHIO
271	CHCL3	112		-0.20	0.42 N	C2H4N2S2	OXAMIDE,DITHIO
272	DIETHYL ETHER	2		-2.54	-1.41 B	C2H4N4	CYANOGUANIDINE/DICYANODIAMIDE/
273	DIETHYL ETHER	3		-2.54	-1.41 B	C2H4N4	CYANOGUANIDINE/DICYANODIAMIDE/
274	OILS	2		-3.33	-1.81 A	C2H4N4	CYANOGUANIDINE/DICYANODIAMIDE/
275	OCTANOL	217	32	-0.90	-0.90 =	C2H4N4O2S2	2-AMINO-1,3,4-THIADIAZOLE-5-SULFONAMIDE
276	CHCL3	217	32	-3.79		C2H4N4O2S2	2-AMINO-1,3,4-THIADIAZOLE-5-SULFONAMIDE
277	DIETHYL ETHER	174		-0.48	0.43 B	C2H4O1	ACETALDEHYDE
278	CHCL3	174		0.11		C2H4O1	ACETALDEHYDE
279	DIETHYL ETHER	112		0.74	0.76 A	C2H4O1S1	THIOACETIC ACID
280	DIETHYL ETHER	46		0.18	0.28 A	C2H4O1S1	THIOACETIC ACID
281	CHCL3	112		0.87	1.41 N	C2H4O1S1	THIOACETIC ACID
282	OCTANOL	218		-0.17	-0.17 =	C2H4O2	ACETIC ACID
283	OCTANOL	5		-0.31	-0.31 =	C2H4O2	ACETIC ACID
284	DIETHYL ETHER	190		-0.35	-0.19 A	C2H4O2	ACETIC ACID
285	DIETHYL ETHER	3		-0.30	-0.15 A	C2H4O2	ACETIC ACID
286	DIETHYL ETHER	177		-0.33	-0.18 A	C2H4O2	ACETIC ACID
287	DIETHYL ETHER	112		-0.36	-0.20 A	C2H4O2	ACETIC ACID
288	DIETHYL ETHER	46		-0.30	-0.15 A	C2H4O2	ACETIC ACID
289	DIETHYL ETHER	40		-0.34	-0.18 A	C2H4O2	ACETIC ACID
290	DIETHYL ETHER	66		-0.34	-0.17 A	C2H4O2	ACETIC ACID
291	DIETHYL ETHER	36		-0.34	-0.18 A	C2H4O2	ACETIC ACID
292	CHCL3	51		-1.19	0.15 A	C2H4O2	ACETIC ACID
293	CHCL3	45		-1.54	-0.09 A	C2H4O2	ACETIC ACID
294	CHCL3	112		-1.52	-0.16 A	C2H4O2	ACETIC ACID
295	CHCL3	46		-1.60	-0.24 A	C2H4O2	ACETIC ACID
296	CHCL3	40		-1.70	-0.31 A	C2H4O2	ACETIC ACID
297	CHCL3	219		-1.58	-0.20 A	C2H4O2	ACETIC ACID
298	OILS	209		-1.30	0.06 A	C2H4O2	ACETIC ACID
299	OILS	220		-1.52	0.19 A	C2H4O2	ACETIC ACID
300	OILS	193		-1.57	-0.25 A	C2H4O2	ACETIC ACID

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
301	BENZENE	51		-1.97	-0.56 A	C2H4O2	ACETIC ACID
302	BENZENE	45		-1.80	-0.32 A	C2H4O2	ACETIC ACID
303	BENZENE	14		-2.00	-0.59 A	C2H4O2	ACETIC ACID
304	BENZENE	40	12	-2.20	-0.79 A	C2H4O2	ACETIC ACID
305	BENZENE	16		-2.05	-0.64 A	C2H4O2	ACETIC ACID
306	BENZENE	66		-1.74	-0.33 A	C2H4O2	ACETIC ACID
307	N-BUTANOL	190		0.09	-0.40	C2H4O2	ACETIC ACID
308	I-BUTANOL	184		0.07	-0.42 A	C2H4O2	ACETIC ACID
309	SEC-BUTANOL	190		0.08	0.40	C2H4O2	ACETIC ACID
310	XYLENE	42		-1.92	-0.29 A	C2H4O2	ACETIC ACID
311	TOLUENE	42		-1.90	-0.09 A	C2H4O2	ACETIC ACID
312	NITROBENZENE	14		-1.44	-0.32	C2H4O2	ACETIC ACID
313	NITROBENZENE	48		-1.42	-0.32	C2H4O2	ACETIC ACID
314	PRIM. PENTANOLS	190		-0.02	-0.42	C2H4O2	ACETIC ACID
315	PRIM. PENTANOLS	184		-0.03	-0.34	C2H4O2	ACETIC ACID
316	PRIM. PENTANOLS	182		-0.03	-0.44	C2H4O2	ACETIC ACID
317	PRIM. PENTANOLS	177		-0.04	-0.35	C2H4O2	ACETIC ACID
318	ETHYL ACETATE	194		-0.18	-0.24	C2H4O2	ACETIC ACID
319	CCL4	45		-1.92	0.22 A	C2H4O2	ACETIC ACID
320	CCL4	14		-2.45	-0.23 A	C2H4O2	ACETIC ACID
321	DI-I-PR. ETHER	190		-0.73	-0.31	C2H4O2	ACETIC ACID
322	DI-I-PR. ETHER	221		-0.77	-0.31 A	C2H4O2	ACETIC ACID
323	DI-I-PR. ETHER	40		-0.77	-0.35	C2H4O2	ACETIC ACID
324	DI-I-PR. ETHER	222		-0.61	-0.17	C2H4O2	ACETIC ACID
325	HEXANE	14		-2.84		C2H4O2	ACETIC ACID
326	2-BUTANONE	190		0.08	0.47	C2H4O2	ACETIC ACID
327	ME-I-BUT.KETONE	195		-0.32	-0.35	C2H4O2	ACETIC ACID
328	OLEYL ALCOHOL	5		-0.66	-0.09	C2H4O2	ACETIC ACID
329	O-NITROTOLUENE	48		-1.48		C2H4O2	ACETIC ACID
330	CYCLOHEXANOL	223	12	-0.06	-1.18	C2H4O2	ACETIC ACID
331	S-PENTANOLS	190		0.16	-0.11	C2H4O2	ACETIC ACID
332	S-PENTANOLS	195		-0.03	-0.34	C2H4O2	ACETIC ACID
333	CS2	14		-2.83		C2H4O2	ACETIC ACID
334	CS2	165		-2.62		C2H4O2	ACETIC ACID
335	PARAFFINS	197	12	-1.32		C2H4O2	ACETIC ACID
336	BROMOFORM	47		-1.58		C2H4O2	ACETIC ACID
337	OCTANOL	5		-1.11	-1.11 =	C2H4O3	HYDROXYACETIC ACID/GLYCOLIC ACID/
338	DIETHYL ETHER	192		-1.55	-1.23 A	C2H4O3	HYDROXYACETIC ACID/GLYCOLIC ACID/
339	OLEYL ALCOHOL	5		-1.70	-1.13	C2H4O3	HYDROXYACETIC ACID /GLYCOLIC ACID/
340	OILS	224		1.57	1.74 B	C2H5BR1	ETHYL BROMIDE
341	OILS	224		1.38	1.54 B	C2H5CL1	ETHYL CHLORIDE
342	OCTANOL	186		2.00	2.00 =	C2H5I1	ETHYL IODIDE
343	DIETHYL ETHER	3	50	2.45	2.27 A	C2H5I1	ETHYL IODIDE
344	OCTANOL	56		-0.13	-0.13 =	C2H5N1O1	ACETALDOXIME
345	DIETHYL ETHER	3		-2.60	-1.46 B	C2H5N1O1	ACETAMIDE
346	DIETHYL ETHER	112		-2.60	-1.46 B	C2H5N1O1	ACETAMIDE
347	CHCL3	112		-2.00	-1.26 N	C2H5N1O1	ACETAMIDE
348	OILS	2		-3.08	-1.58 A	C2H5N1O1	ACETAMIDE
349	DIETHYL ETHER	192	12	-2.08	-1.71 A	C2H5N1O2	AMINOACETIC ACID/GLYCINE/
350	N-BUTANOL	225		-1.81	-3.03	C2H5N1O2	AMINOACETIC ACID/GLYCINE/
351	SEC-BUTANOL	84	19	-1.01	-1.92	C2H5N1O2	AMINOACETIC ACID/GLYCINE/
352	S-PENTANOLS	195		-1.82	-2.39	C2H5N1O2	AMINOACETIC ACID/GLYCINE/
353	DIETHYL ETHER	3		-0.85	-0.63 A	C2H5N1O2	O-METHYL CARBAMATE
354	OILS	2		-1.60	-0.26 A	C2H5N1O2	O-METHYL CARBAMATE
355	OILS	224		-1.40	-0.04 A	C2H5N1O2	O-METHYL CARBAMATE
356	OILS	214		-1.40	-0.04 A	C2H5N1O2	O-METHYL CARBAMATE
357	OCTANOL	186		0.18	0.18 =	C2H5N1O2	NITROETHANE
358	DIETHYL ETHER	112		-0.55	0.36 B	C2H5N1S1	THIOACETAMIDE
359	CHCL3	112		-1.14	-0.46 N	C2H5N1S1	THIOACETAMIDE
360	OCTANOL	226		-0.16	-0.16 =	C2H5N3O2	1-METHYL-1-NITROSOUREA (23909)
361	OCTANOL	227		-0.03	-0.03 =	C2H5N3O2	1-METHYL-1-NITROSOUREA (23909)
362	CCL4	228		-0.04	-0.09 B	C2H6F1O3P1	DIMETHYLFLUOROPHOSPHATE
363	DIETHYL ETHER	3		-2.92	-1.75 A	C2H6N2O1	METHYL UREA
364	OILS	2		-3.36	-1.84 A	C2H6N2O1	METHYL UREA
365	DIETHYL ETHER	3		-3.55	-2.98 A	C2H6N2O2	METHYLOLUREA
366	DIETHYL ETHER	198		-1.64	-1.31 A	C2H6N2S1	METHYLTHIOUREA
367	OCTANOL	5		-0.32	-0.32 =	C2H6O1	ETHANOL
368	DIETHYL ETHER	3		-0.58	-0.39 A	C2H6O1	ETHANOL
369	DIETHYL ETHER	198	12	0.28	0.37 A	C2H6O1	ETHANOL
370	DIETHYL ETHER	174		-0.57	-0.38 A	C2H6O1	ETHANOL
371	CYCLOHEXANE	82		-2.37		C2H6O1	ETHANOL
372	CYCLOHEXANE	229		-1.96		C2H6O1	ETHANOL
373	CHCL3	174		-0.85	-0.18 N	C2H6O1	ETHANOL
374	OILS	230		-1.52	-0.19 A	C2H6O1	ETHANOL
375	OILS	173		-1.45	-0.13 A	C2H6O1	ETHANOL
376	OILS	101		-1.45	-0.11 A	C2H6O1	ETHANOL
377	OILS	200		-1.49	-0.17 A	C2H6O1	ETHANOL
378	OILS	70		-1.33	0.00 A	C2H6O1	ETHANOL
379	BENZENE	82		-1.58	-0.18 A	C2H6O1	ETHANOL
380	BENZENE	231		-1.49	-0.09	C2H6O1	ETHANOL
381	BENZENE	232	12	-0.01	1.37 A	C2H6O1	ETHANOL
382	CCL4	233	12	-1.61	0.47 A	C2H6O1	ETHANOL
383	HEXANE	82		-2.26		C2H6O1	ETHANOL
384	OLEYL ALCOHOL	82		-1.00	-0.43	C2H6O1	ETHANOL
385	CS2	233		-1.84		C2H6O1	ETHANOL
386	OCTANOL	9		-2.03	-2.03 =	C2H6O1S1	DIMETHYLSULFOXIDE
387	CCL4	234	12	-1.51		C2H6O1S1	DIMETHYLSULFOXIDE
388	OCTANOL	9		-1.93	-1.93 =	C2H6O2	ETHANE-1,2-DIOL/ETHYLENE GLYCOL/
389	DIETHYL ETHER	3		-2.27	-1.88 A	C2H6O2	ETHANE-1,2-DIOL/ETHYLENE GLYCOL/
390	OILS	2		-3.31	-1.79 A	C2H6O2	ETHANE-1,2-DIOL/ETHYLENE GLYCOL/
391	OCTANOL	235		1.77	1.77 =	C2H6S2	DIMETHYLDISULFIDE
392	DIETHYL ETHER	3		-1.22	-0.23 B	C2H7N1	DIMETHYLAMINE
393	BENZENE	205		-0.82	-0.02	C2H7N1	DIMETHYLAMINE
394	1-BUTANOL	184		0.10	-0.38	C2H7N1	DIMETHYLAMINE
395	XYLENE	46		-0.68	-0.10 B	C2H7N1	DIMETHYLAMINE
396	TOLUENE	205		-1.08	-0.12 B	C2H7N1	DIMETHYLAMINE
397	TOLUENE	68		-1.28	-0.27 B	C2H7N1	DIMETHYLAMINE
398	DIETHYL ETHER	3		-1.18	-0.19 B	C2H7N1	ETHYLAMINE
399	XYLENE	46		-0.66	-0.08 B	C2H7N1	ETHYLAMINE
400	TOLUENE	68		-1.28	-0.27 B	C2H7N1	ETHYLAMINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
401	OCTANOL	5		-1.31	-1.31 =	C2H7N1O1	ETHANOLAMINE
402	DIETHYL ETHER	3	50	-2.89	-1.71 B	C2H7N1O1	ETHANOLAMINE
403	PRIM. PENTANOLS	236	17	-0.18	-0.53	C2H7O4P1	PHOSPHATE,MONOETHYL
404	OCTANOL	206		1.96	1.96 =	C3H1BR3N2	IMIDAZOLE,2,4,5-TRIBROMO
405	OCTANOL	206		1.18	1.18 =	C3H1CL3N2	IMIDAZOLE,2,4,5-TRICHLORO
406	OCTANOL	206		2.78	2.78 =	C3H1I3N2	IMIDAZOLE,2,4,5-TRIIODO
407	DIETHYL ETHER	237		0.04	0.15 A	C3H2N2	MALONONITRILE
408	CHCL3	237		-0.53	0.11 N	C3H2N2	MALONONITRILE
409	DIETHYL ETHER	112		0.40	0.46 A	C3H2O2	ACETYLENE CARBOXYLIC ACID/PROPIOLIC ACID/
410	CHCL3	112		-1.85	-0.46 A	C3H2O2	ACETYLENE CARBOXYLIC ACID/PROPIOLIC ACID/)
411	OCTANOL	9		1.23	1.23 =	C3H3F5O1	PROPANOL, 2,2,3,3,3-PENTAFLUORO
412	OCTANOL	5		-0.92	-0.92 =	C3H3N1	ACRYLONITRILE
413	OCTANOL	56		0.08	0.08 =	C3H3N1O1	ISOXAZOLE
414	DIETHYL ETHER	207		-0.52	-0.33 A	C3H3N1O2	CYANOACETIC ACID
415	DIETHYL ETHER	112		-0.43	-0.26 A	C3H3N1O2	CYANOACETIC ACID
416	DIETHYL ETHER	66		-0.44	-0.26 A	C3H3N1O2	CYANOACETIC ACID
417	CHCL3	112		-2.17	-0.75 A	C3H3N1O2	CYANOACETIC ACID
418	BENZENE	66	12	-0.76	0.63 A	C3H3N1O2	CYANOACETIC ACID
419	OCTANOL	218		0.44	0.44 =	C3H3N1S1	THIAZOLE
420	OCTANOL	218		0.22	0.22 =	C3H3N3O2	AZAURACIL
421	DIETHYL ETHER	207		0.68	0.72 A	C3H4BR2O2	A,B-DIBROMOPROPIONIC ACID
422	DIETHYL ETHER	46	12	1.79	1.69 A	C3H4BR2O2	A,B-DIBROMOPROPIONIC ACID
423	CHCL3	46		-0.42	0.84 A	C3H4BR2O2	A,B-DIBROMOPROPIONIC ACID
424	XYLENE	46		-0.60	1.13 A	C3H4BR2O2	A,B-DIBROMOPROPIONIC ACID
425	OILS	173		-0.28	0.21 B	C3H4CL2O1	1,3-DICHLOROACETONE
426	OCTANOL	238		0.13	0.13 =	C3H4N2	PYRAZOLE
427	OCTANOL	56		-1.69	-1.69 =	C3H4N2O2	HYDANTOIN
428	DIETHYL ETHER	192		0.36	0.43 A	C3H4O2	ACRYLIC ACID
429	ME-I-BUT.KETONE	195		0.40	0.31	C3H4O2	ACRYLIC ACID
430	DIETHYL ETHER	112		-0.62	-0.43 A	C3H4O3	A-KETOPROPIONIC ACID/PYRUVIC ACID/
431	DIETHYL ETHER	46		-0.41	-0.24 A	C3H4O3	A-KETOPROPIONIC ACID/PYRUVIC ACID/
432	CHCL3	112		-2.18	-0.75 A	C3H4O3	A-KETOPROPIONIC ACID/PYRUVIC ACID/
433	CHCL3	46		-1.02	0.29 A	C3H4O3	A-KETOPROPIONIC ACID/PYRUVIC ACID/
434	XYLENE	46		-1.52	0.13 A	C3H4O3	A-KETOPROPIONIC ACID/PYRUVIC ACID/
435	OLEYL ALCOHOL	5		-0.92	-0.35	C3H4O3	A-KETOPROPIONIC ACID/PYRUVIC ACID/
436	DIETHYL ETHER	212		-0.99	-0.75 A	C3H4O4	MALONIC ACID
437	DIETHYL ETHER	207		-1.08	-0.81 A	C3H4O4	MALONIC ACID
438	DIETHYL ETHER	194		-0.91	-0.68 A	C3H4O4	MALONIC ACID
439	DIETHYL ETHER	46		-0.34	-0.18 A	C3H4O4	MALONIC ACID
440	DIETHYL ETHER	64		-0.89	-0.66 A	C3H4O4	MALONIC ACID
441	N-BUTANOL	194		-0.28	-0.91	C3H4O4	MALONIC ACID
442	1-BUTANOL	48		-0.11	-0.66	C3H4O4	MALONIC ACID
443	PRIM. PENTANOLS	48		-0.22	-0.58	C3H4O4	MALONIC ACID
444	ETHYL ACETATE	194		-0.65	-0.75	C3H4O4	MALONIC ACID
445	HEXANOL	74		-0.51		C3H4O4	MALONIC ACID
446	ME-I-BUT.KETONE	195		-0.73	-0.68	C3H4O4	MALONIC ACID
447	OLEYL ALCOHOL	5		-1.28	-0.70	C3H4O4	MALONIC ACID
448	S-PENTANOLS	195		-0.43	-0.80	C3H4O4	MALONIC ACID
449	N-BUTANOL	181	10	-0.40		C3H4O7P1	PHOSPHOGLYCERATE ANION
450	PRIM. PENTANOLS	181	10	0.11		C3H4O7P1	PHOSPHOGLYCERATE ANION
451	HEXANOL	181	18	-0.52		C3H4O7P1	PHOSPHOGLYCERATE ANION
452	OCTANOL	5		0.92	0.92 =	C3H5BR1O2	A-BROMOPROPIONIC ACID
453	DIETHYL ETHER	3		1.18	1.15 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
454	DIETHYL ETHER	207		1.04	1.03 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
455	DIETHYL ETHER	46		1.50	1.44 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
456	CHCL3	29		-0.44	0.82 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
457	OILS	209		-0.18	1.08 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
458	BENZENE	29		-0.62	0.76 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
459	XYLENE	46		-1.01	0.69 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
460	TOLUENE	29		-0.80	0.86 A	C3H5BR1O2	A-BROMOPROPIONIC ACID
461	CHCL3	29		-0.61	0.65 A	C3H5BR1O2	B-BROMOPROPIONIC ACID
462	OILS	209		-0.34	0.91 A	C3H5BR1O2	B-BROMOPROPIONIC ACID
463	BENZENE	29		-0.85	0.54 A	C3H5BR1O2	B-BROMOPROPIONIC ACID
464	TOLUENE	29		-0.97	0.71 A	C3H5BR1O2	B-BROMOPROPIONIC ACID
465	OILS	239		2.16	2.14 B	C3H5CL1N2O6	2,3-PROPANEDIOL DINITRATE,1-CHLORO
466	OILS	173		0.03	0.28 B	C3H5CL1O1	CHLOROACETONE
467	DIETHYL ETHER	207		0.95	0.96 A	C3H5CL1O2	A-CHLOROPROPIONIC ACID
468	DIETHYL ETHER	207		0.62	0.66 A	C3H5CL1O2	B-CHLOROPROPIONIC ACID
469	CHCL3	29		-0.86	0.44 A	C3H5CL1O2	B-CHLOROPROPIONIC ACID
470	OILS	209		-0.53	0.76 A	C3H5CL1O2	B-CHLOROPROPIONIC ACID
471	BENZENE	29		-1.06	0.33 A	C3H5CL1O2	B-CHLOROPROPIONIC ACID
472	TOLUENE	29		-1.23	0.49 A	C3H5CL1O2	B-CHLOROPROPIONIC ACID
473	CHCL3	29		-0.40	0.85 A	C3H5I1O2	B-IODOPROPIONIC ACID
474	CHCL3	46		-0.32	0.93 A	C3H5I1O2	B-IODOPROPIONIC ACID
475	BENZENE	29		-0.52	0.86 A	C3H5I1O2	B-IODOPROPIONIC ACID
476	XYLENE	46		-0.82	0.89 A	C3H5I1O2	B-IODOPROPIONIC ACID
477	TOLUENE	29		-0.68	0.95 A	C3H5I1O2	B-IODOPROPIONIC ACID
478	DIETHYL ETHER	46		1.15	1.13 A	C3H5I1O2	B-IODOPROPIONIC ACIDD
479	OCTANOL	186		0.16	0.16 =	C3H5N1	PROPIONITRILE
480	OCTANOL	5		0.04	0.04 =	C3H5N1	PROPIONITRILE
481	OILS	239		2.04	2.05 B	C3H5N3O9	GLYCERYL TRINITRATE
482	OILS	240		2.06	2.35 B	C3H5N3O9	GLYCERYL TRINITRATE
483	OCTANOL	227		0.57	0.57 =	C3H6CL1N3O2	1-(2-CHLOROETHYL)-1-NITROSOUREA (NCS 47547)
484	DIETHYL ETHER	2		-0.34	-0.18 A	C3H6N2	DIMETHYL CYANAMIDE
485	OILS	2		-1.14	-0.50 B	C3H6N2	DIMETHYL CYANAMIDE
486	DIETHYL ETHER	3	12	-3.52	-2.87 A	C3H6N2O2	MALONDIAMIDE
487	I-BUTANOL	4		-1.06	-1.99	C3H6N2O2	MALONDIAMIDE
488	OCTANOL	238		-0.66	-0.66 =	C3H6N2S1	IMIDAZOLIDONE,2-THIO/ETHYLENETHIOUREA/
489	PARAFFINS	241		-1.79		C3H6N2S1	IMIDAZOLIDONE,2-THIO/ETHYLENETHIOUREA/
490	OCTANOL	5		-0.24	-0.24 =	C3H6O1	ACETONE
491	DIETHYL ETHER	3	50	-0.21	-0.06 A	C3H6O1	ACETONE
492	CYCLOHEXANE	242		-0.96		C3H6O1	ACETONE
493	CHCL3	243	12	0.72	0.39 B	C3H6O1	ACETONE
494	OILS	230		-0.70	-0.14 B	C3H6O1	ACETONE
495	OILS	173		-1.10	-0.47 B	C3H6O1	ACETONE
496	OILS	70		-0.64	-0.09 B	C3H6O1	ACETONE
497	BENZENE	51	12	-0.04	0.52 B	C3H6O1	ACETONE
498	BENZENE	182	12	-0.03	0.51 B	C3H6O1	ACETONE
499	BENZENE	244	12	-0.04	0.52 B	C3H6O1	ACETONE
500	BENZENE	42	12	0.00	0.55 B	C3H6O1	ACETONE

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501	TOLUENE	188	12	-0.31	0.43 B	C3H6O1	ACETONE
502	CCL4	51	12	-0.37		C3H6O1	ACETONE
503	CCL4	243		-0.35	-0.25 B	C3H6O1	ACETONE
504	CCL4	37		-0.34	-0.36 B	C3H6O1	ACETONE
505	HEXANE	242		-0.92		C3H6O1	ACETONE
506	CS2	242		-0.52		C3H6O1	ACETONE
507	CL3CCHCL2	243		0.22		C3H6O1	ACETONE
508	CL2CHCHCL2	243		0.63		C3H6O1	ACETONE
509	CL2C=CCL2	243		-0.55		C3H6O1	ACETONE
510	CL2C=CHCL	243		0.05		C3H6O1	ACETONE
511	OCTANOL	56		0.17	0.17 =	C3H6O1	ALLYL ALCOHOL
512	DIETHYL ETHER	174		-0.12	0.02 A	C3H6O1	ALLYL ALCOHOL
513	CHCL3	174		-0.51	0.13 N	C3H6O1	ALLYL ALCOHOL
514	DIETHYL ETHER	3		0.30	0.38 A	C3H6O1	PROPIONALDEHYDE
515	OCTANOL	5		0.18	0.18 =	C3H6O2	ACETIC ACID, METHYL ESTER
516	DIETHYL ETHER	3	50	0.43	0.49 A	C3H6O2	ACETIC ACID,METHYL ESTER
517	OILS	2		-0.37	0.20 B	C3H6O2	ACETIC ACID,METHYL ESTER
518	BENZENE	245	12	0.47	0.87 B	C3H6O2	ACETIC ACID,METHYL ESTER
519	CCL4	245		0.41	0.32 B	C3H6O2	ACETIC ACID,METHYL ESTER
520	CS2	245		0.26		C3H6O2	ACETIC ACID,METHYL ESTER
521	OCTANOL	218		0.33	0.33 =	C3H6O2	PROPIONIC ACID
522	OCTANOL	5		0.25	0.25 =	C3H6O2	PROPIONIC ACID
523	DIETHYL ETHER	190		0.13	0.23 A	C3H6O2	PROPIONIC ACID
524	DIETHYL ETHER	207		0.20	0.29 A	C3H6O2	PROPIONIC ACID
525	DIETHYL ETHER	112		0.23	0.31 A	C3H6O2	PROPIONIC ACID
526	DIETHYL ETHER	46		0.18	0.27 A	C3H6O2	PROPIONIC ACID
527	DIETHYL ETHER	49		0.23	0.33 A	C3H6O2	PROPIONIC ACID
528	DIETHYL ETHER	36		0.27	0.35 A	C3H6O2	PROPIONIC ACID
529	CHCL3	51		-0.78	0.52 A	C3H6O2	PROPIONIC ACID
530	CHCL3	14		-0.79	0.51 A	C3H6O2	PROPIONIC ACID
531	CHCL3	48		-0.79	0.50 A	C3H6O2	PROPIONIC ACID
532	CHCL3	112		-0.85	0.45 A	C3H6O2	PROPIONIC ACID
533	CHCL3	29		-0.80	0.49 A	C3H6O2	PROPIONIC ACID
534	OILS	209		-0.80	0.51 A	C3H6O2	PROPIONIC ACID
535	OILS	193		-0.85	0.42 A	C3H6O2	PROPIONIC ACID
536	BENZENE	51		-1.20	0.25 A	C3H6O2	PROPIONIC ACID
537	BENZENE	44		-1.16	0.24 A	C3H6O2	PROPIONIC ACID
538	BENZENE	14		-1.37	0.03 A	C3H6O2	PROPIONIC ACID
539	BENZENE	29		-1.22	0.18 A	C3H6O2	PROPIONIC ACID
540	N-BUTANOL	190		0.51	0.19	C3H6O2	PROPIONIC ACID
541	I-BUTANOL	184		0.51	0.22	C3H6O2	PROPIONIC ACID
542	1-BUTANOL	48		0.43	0.10	C3H6O2	PROPIONIC ACID
543	SEC-BUTANOL	190		0.39	0.44	C3H6O2	PROPIONIC ACID
544	XYLENE	48		-1.32		C3H6O2	PROPIONIC ACID
545	XYLENE	46		-1.24	0.44 A	C3H6O2	PROPIONIC ACID
546	TOLUENE	51		-1.34	0.39 A	C3H6O2	PROPIONIC ACID
547	TOLUENE	29		-1.33	0.40 A	C3H6O2	PROPIONIC ACID
548	NITROBENZENE	14		-0.80	0.21	C3H6O2	PROPIONIC ACID
549	NITROBENZENE	48		-0.75	0.28	C3H6O2	PROPIONIC ACID
550	PRIM. PENTANOLS	190		0.54	0.30	C3H6O2	PROPIONIC ACID
551	PRIM. PENTANOLS	48		0.37	0.16	C3H6O2	PROPIONIC ACID
552	ETHYL ACETATE	194		0.35	0.32	C3H6O2	PROPIONIC ACID
553	CCL4	14		-1.79	0.33 A	C3H6O2	PROPIONIC ACID
554	CCL4	48		-1.62	0.46 A	C3H6O2	PROPIONIC ACID
555	DI-I-PR. ETHER	190		-0.09	0.44	C3H6O2	PROPIONIC ACID
556	DI-I-PR. ETHER	221		-0.09	0.41	C3H6O2	PROPIONIC ACID
557	DI-I-PR. ETHER	222		-0.01	0.47	C3H6O2	PROPIONIC ACID
558	2-BUTANONE	190		0.40	0.14	C3H6O2	PROPIONIC ACID
559	ME-I-BUT.KETONE	195		0.21	0.14	C3H6O2	PROPIONIC ACID
560	OLEYL ALCOHOL	5		-0.09	0.46	C3H6O2	PROPIONIC ACID
561	ETHYL BROMIDE	48		-0.70		C3H6O2	PROPIONIC ACID
562	O-NITROTOLUENE	48		-0.86		C3H6O2	PROPIONIC ACID
563	DECALIN	48		-1.44		C3H6O2	PROPIONIC ACID
564	S-PENTANOLS	190		0.58	0.36	C3H6O2	PROPIONIC ACID
565	S-PENTANOLS	195		0.49	0.25	C3H6O2	PROPIONIC ACID
566	PARAFFINS	14		-2.15		C3H6O2	PROPIONIC ACID
567	PARAFFINS	197	12	-1.28		C3H6O2	PROPIONIC ACID
568	DECALIN	246		-1.56		C3H6O2	PROPIONIC ACID
569	OCTANOL	5		-0.62	-0.62 =	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
570	DIETHYL ETHER	51		-1.09	-0.84 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
571	DIETHYL ETHER	247		-0.99	-0.74 A	C3H6O3	A-HYDROXYPROPIONIC ACID /LACTIC ACID/
572	DIETHYL ETHER	112		-0.96	-0.73 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
573	DIETHYL ETHER	46		-0.64	-0.44 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
574	DIETHYL ETHER	49		-1.09	-0.84 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
575	DIETHYL ETHER	213		-1.07	-0.82 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
576	CHCL3	112		-2.23	-0.81 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
577	CHCL3	46		-1.81	-0.43 A	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
578	I-BUTANOL	184		-0.10	-0.65	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
579	PRIM. PENTANOLS	247		-0.32	-0.81	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
580	PRIM. PENTANOLS	48		-0.40	-0.81	C3H6O3	A-HYDROXYPROPIONIC ACID /LACTIC ACID/
581	ME-I-BUT.KETONE	195		-0.80	-0.74	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
582	OLEYL ALCOHOL	5		-1.21	-0.64	C3H6O3	A-HYDROXYPROPIONIC ACID /LACTIC ACID/
583	S-PENTANOLS	195		-0.31	-0.66	C3H6O3	A-HYDROXYPROPIONIC ACID/LACTIC ACID/
584	DIETHYL ETHER	207		-0.76	-0.55 A	C3H6O3	METHOXYACETIC ACID
585	DIETHYL ETHER	112		-0.62	-0.43 A	C3H6O3	METHOXYACETIC ACID
586	CHCL3	112	12	-1.30	0.04 A	C3H6O3	METHOXYACETIC ACID
587	ME-I-BUT.KETONE	195		-0.57	-0.58	C3H6O3	METHOXYACETIC ACID
588	S-PENTANOLS	195		-0.30	-0.65	C3H6O3	METHOXYACETIC ACID
589	DIETHYL ETHER	3		-2.05	-1.68 A	C3H6O4	A,B-DIHYDROXYPROPIONIC ACID/GLYCERIC ACID/
590	OCTANOL	186		2.10	2.10 =	C3H7BR1	1-BROMOPROPANE
591	DIETHYL ETHER	2		-1.10	-0.85 A	C3H7CL1O2	GLYCEROL MONOCHLOROHYDRIN
592	OILS	2		-1.92	-0.55 A	C3H7CL1O2	GLYCEROL MONOCHLOROHYDRIN
593	DIETHYL ETHER	3		-1.10	-0.85 A	C3H7CL1O2	GLYCEROL-A-MONOCHLOROHYDRIN
594	DIETHYL ETHER	2		-1.62	-0.59 B	C3H7N1O1	DIMETHYLFORMAMIDE
595	OILS	2		-2.31	-0.87 A	C3H7N1O1	DIMETHYLFORMAMIDE
596	OCTANOL	235		-1.05	-1.05 =	C3H7N1O1	N-METHYLACETAMIDE
597	DIETHYL ETHER	3		-1.89	-0.81 B	C3H7N1O1	PROPIONAMIDE
598	CHCL3	248		-1.40	-0.70 N	C3H7N1O1	PROPIONAMIDE
599	OILS	2		-2.44	-0.99 A	C3H7N1O1	PROPIONAMIDE
600	DIETHYL ETHER	3	50	-1.14	-0.88 A	C3H7N1O2	AMINOACETIC ACID, METHYL ESTER

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
601	OCTANOL	56		-2.94	-2.94 =	C3H7N1O2	A-AMINOPROPIONIC ACID/ALANINE/
602	DIETHYL ETHER	3	12	-5.85	-5.00 A	C3H7N1O2	A-AMINOPROPIONIC ACID/ALANINE/
603	N-BUTANOL	225		-1.60	-2.74	C3H7N1O2	A-AMINOPROPIONIC ACID /ALANINE/
604	SEC-BUTANOL	84	19	-0.94	-1.82	C3H7N1O2	A-AMINOPROPIONIC ACID /ALANINE/
605	OCTANOL	218		-0.15	-0.15 =	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
606	DIETHYL ETHER	3		-0.19	-0.04 A	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
607	OILS	2		-1.12	0.22 A	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
608	OILS	173		-0.92	0.38 A	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
609	OILS	82		-1.52	-0.15 A	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
610	OILS	214		-0.85	0.44 A	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
611	OILS	249		-1.00	0.30 A	C3H7N1O2	O-ETHYL CARBAMATE/URETHANE/
612	DIETHYL ETHER	3		-2.74	-2.28 A	C3H7N1O2	A-HYDROXYPROPIONAMIDE/LACTAMIDE/
613	OCTANOL	186		0.65	0.65 =	C3H7N1O2	1-NITROPROPANE
614	CYCLOHEXANE	250		0.53		C3H7N1O2	1-NITROPROPANE
615	CHCL3	250	12	1.91	2.41 N	C3H7N1O2	1-NITROPROPANE
616	TOLUENE	250		1.40	1.67 B	C3H7N1O2	1-NITROPROPANE
617	CCL4	250		0.99		C3H7N1O2	1-NITROPROPANE
618	OCTANE	250		0.45		C3H7N1O2	1-NITROPROPANE
619	CS2	250		0.85		C3H7N1O2	1-NITROPROPANE
620	OILS	240		0.45	1.46 A	C3H7N1O5	GLYCERYL MONONITRATE
621	OCTANOL	181	10	0.28	0.28 =	C3H7O6P1	B-GLYCEROPHOSPHATE ANION
622	N-BUTANOL	181	10	-0.70		C3H7O6P1	B-GLYCEROPHOSPHATE ANION
623	PRIM. PENTANOLS	181	10	0.04		C3H7O6P1	B-GLYCEROPHOSPHATE ANION
624	HEXANOL	181	18	-0.04		C3H7O6P1	B-GLYCEROPHOSPHATE ANION
625	OCTANOL	181	10	0.43	0.43 =	C3H7O6P1	L-A-GLYCEROPHOSPHATE ANION
626	N-BUTANOL	181	10	-0.70		C3H7O6P1	L-A-GLYCEROPHOSPHATE ANION
627	PRIM. PENTANOLS	181	10	0.21		C3H7O6P1	L-A-GLYCEROPHOSPHATE ANION
628	HEXANOL	181	18	0.18		C3H7O6P1	L-A-GLYCEROPHOSPHATE ANION
629	PRIM. PENTANOLS	181	10	-0.22		C3H8N1O6P1	SERINE PHOSPHATE
630	OILS	2		-2.64	-1.17 A	C3H8N2O1	N,N-DIMETHYLUREA
631	DIETHYL ETHER	3		-2.51	-2.07 A	C3H8N2O1	DIMETHYLUREA,SYM.
632	DIETHYL ETHER	3		-2.54	-2.10 A	C3H8N2O1	DIMETHYLUREA,UNSYM
633	DIETHYL ETHER	3		-2.39	-1.97 A	C3H8N2O1	ETHYLUREA
634	OILS	2		-2.77	-1.29 A	C3H8N2O1	ETHYLUREA
635	DIETHYL ETHER	198		-1.35	-1.06 A	C3H8N2S1	ETHYLTHIOUREA
636	OCTANOL	186		0.34	0.34 =	C3H8O1	PROPANOL
637	DIETHYL ETHER	3		0.28	0.36 A	C3H8O1	PROPANOL
638	DIETHYL ETHER	174		-0.03	0.10 A	C3H8O1	PROPANOL
639	CYCLOHEXANE	82		-1.49		C3H8O1	PROPANOL
640	CHCL3	174		-0.21	0.41 N	C3H8O1	PROPANOL
641	OILS	173		-0.85	0.42 A	C3H8O1	PROPANOL
642	OILS	101		-0.81	0.45 A	C3H8O1	PROPANOL
643	OILS	200		-0.89	0.38 A	C3H8O1	PROPANOL
644	OILS	201		-0.81	0.45 A	C3H8O1	PROPANOL
645	BENZENE	82		-0.87	0.48 A	C3H8O1	PROPANOL
646	BENZENE	231		-0.65	0.74	C3H8O1	PROPANOL
647	HEXANE	82		-1.48		C3H8O1	PROPANOL
648	OLEYL ALCOHOL	82		-0.45	0.12	C3H8O1	PROPANOL
649	DIETHYL ETHER	2		-0.19	-0.04 A	C3H8O1	1-PROPANOL
650	DIETHYL ETHER	174		-0.33	-0.16 A	C3H8O1	1-PROPANOL
651	CHCL3	174		-0.35	0.28 N	C3H8O1	1-PROPANOL
652	OILS	2		-1.32	0.00 A	C3H8O1	1-PROPANOL
653	OILS	201		-1.05	0.24 A	C3H8O1	1-PROPANOL
654	OCTANOL	5		0.00	0.00 =	C3H8O2	DIMETHOXYMETHANE
655	DIETHYL ETHER	3		-0.82	-0.60 A	C3H8O2	METHOXYETHANOL
656	OILS	2		-2.25	-0.82 A	C3H8O2	METHOXYETHANOL
657	DIETHYL ETHER	3		-1.74	-1.41 A	C3H8O2	1,2-PROPANEDIOL
658	OILS	2		-2.77	-1.30 A	C3H8O2	1,2-PROPANEDIOL
659	DIETHYL ETHER	3		-2.00	-1.64 A	C3H8O2	TRIMETHYLENE GLYCOL
660	DIETHYL ETHER	3		-3.18	-2.66 A	C3H8O3	GLYCEROL
661	DIETHYL ETHER	198		-2.96	-2.47 A	C3H8O3	GLYCEROL
662	OILS	2		-4.15	-2.56 A	C3H8O3	GLYCEROL
663	OCTANOL	218		-0.03	-0.03 =	C3H9N1	ISOPROPYLAMINE
664	DIETHYL ETHER	3		-0.54	0.37 B	C3H9N1	PROPYLAMINE
665	XYLENE	46		-0.36	0.21 B	C3H9N1	PROPYLAMINE
666	TOLUENE	68		-0.65	0.15 B	C3H9N1	PROPYLAMINE
667	OCTANOL	251		0.27	0.27 =	C3H9N1	TRIMETHYLAMINE
668	DIETHYL ETHER	3		-0.34	0.54 B	C3H9N1	TRIMETHYLAMINE
669	DIETHYL ETHER	251		-0.26	0.61 B	C3H9N1	TRIMETHYLAMINE
670	DIETHYL ETHER	188		-0.38	0.52 B	C3H9N1	TRIMETHYLAMINE
671	CYCLOHEXANE	251		-0.44		C3H9N1	TRIMETHYLAMINE
672	CHCL3	251		0.54	0.23 B	C3H9N1	TRIMETHYLAMINE
673	CHCL3	46		0.59	0.27 B	C3H9N1	TRIMETHYLAMINE
674	BENZENE	205		-0.33	0.31 B	C3H9N1	TRIMETHYLAMINE
675	BENZENE	251		-0.29	0.35 B	C3H9N1	TRIMETHYLAMINE
676	1-BUTANOL	184		0.49	0.18	C3H9N1	TRIMETHYLAMINE
677	XYLENE	205		-0.44	1.45 B	C3H9N1	TRIMETHYLAMINE
678	TOLUENE	205		-0.36	0.40 B	C3H9N1	TRIMETHYLAMINE
679	TOLUENE	68		-0.36	0.40 B	C3H9N1	TRIMETHYLAMINE
680	TOLUENE	188		-0.34	0.42 B	C3H9N1	TRIMETHYLAMINE
681	CCL4	251		-0.09	0.66 N	C3H9N1	TRIMETHYLAMINE
682	DI-I-PR. ETHER	251		-0.36	0.10	C3H9N1	TRIMETHYLAMINE
683	OCTANOL	5		-0.96	-0.96 =	C3H9N1O1	2-PROPANOL,1-AMINO
684	DIETHYL ETHER	3	50	-2.37	-1.22 B	C3H9N1O1	2-PROPANOL,1-AMINO
685	PRIM. PENTANOLS	236	17	-0.06	-0.38	C3H9O4P1	PHOSPHATE,MONO-N-PROPYL
686	OCTANOL	56		-0.52	-0.52 =	C3H9O4P1	PHOSPHORIC ACID, TRIMETHYL ESTER
687	DIETHYL ETHER	3		-2.94	-1.77 B	C3H10N2	1,2-PROPYLENEDIAMINE
688	1-BUTANOL	4		-0.92	-1.80	C3H10N2O1	1,3-DIAMINOPROPANOL-2
689	DIETHYL ETHER	3		-3.70	-2.44 B	C3H10N2O3	1,3-DIAMINO-PROPANOL-2
690	OCTANOL	226		-0.95	-0.95 =	C4H3F1N2O2	5-FLUORDURACIL (19893)
691	OCTANOL	9		1.81	1.81 =	C4H3F7O1	BUTANOL,2,2,3,3,4,4,4-HEPTAFLUORO
692	N-BUTANOL	252	38	0.04	-0.46	C4H3N5O2	AZAXANTHINE
693	DIETHYL ETHER	212		1.73	1.63 A	C4H4BR2O4	1,2-DIBROMOSUCCINIC ACID
694	OCTANOL	238		-0.40	-0.40 =	C4H4N2	PYRIMIDINE
695	CHCL3	188		-0.23	0.35 N	C4H4N2	SUCCINODINITRILE
696	OCTANOL	235	70	-0.28	-0.28 =	C4H4N2O1S1	2-THIOURACIL
697	N-BUTANOL	253	36	-0.40	-1.07	C4H4N2O2	URACIL
698	OCTANOL	218		-1.47	-1.47 =	C4H4N2O3	BARBITURIC ACID
699	DIETHYL ETHER	192		-1.63	-1.32 A	C4H4N2O3	BARBITURIC ACID
700	CHCL3	254		-2.10	-1.32 N	C4H4N2O3	BARBITURIC ACID

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701	N-BUTANOL	253	36	-1.16	-2.12	C4H4N2O3	BARBITURIC ACID
702	OCTANOL	65		-1.66	-1.66 =	C4H4N2O4	3-CARBOXYMETHYLSYONONE
703	OCTANOL	227		-0.71	-0.71 =	C4H4N6O1	8-AZAGUANINE (NCS 749)(PKA= 6.43)
704	DIETHYL ETHER	212		0.19	0.28 A	C4H4O4	FUMARIC ACID
705	DIETHYL ETHER	207		0.10	0.20 A	C4H4O4	FUMARIC ACID
706	DIETHYL ETHER	46		0.07	0.18 A	C4H4O4	FUMARIC ACID
707	1-BUTANOL	4		0.76	0.56	C4H4O4	FUMARIC ACID
708	ETHYL ACETATE	194		0.23	0.23	C4H4O4	FUMARIC ACID
709	CYCLOHEXANONE	194		0.54		C4H4O4	FUMARIC ACID
710	2-BUTANONE	194		0.53	0.41	C4H4O4	FUMARIC ACID
711	ME-I-BUT.KETONE	194		0.08	0.07	C4H4O4	FUMARIC ACID
712	ME-I-BUT.KETONE	195		0.22	0.20	C4H4O4	FUMARIC ACID
713	S-PENTANOLS	195		0.60	0.38	C4H4O4	FUMARIC ACID
714	DIETHYL ETHER	212		-0.82	-0.61 A	C4H4O4	MALEIC ACID
715	DIETHYL ETHER	207		-1.04	-0.79 A	C4H4O4	MALEIC ACID
716	DIETHYL ETHER	46		-0.50	-0.32 A	C4H4O4	MALEIC ACID
717	1-BUTANOL	4		0.11	-0.35	C4H4O4	MALEIC ACID
718	ME-I-BUT.KETONE	195		-0.66	-0.66	C4H4O4	MALEIC ACID
719	OLEYL ALCOHOL	5		-0.89	-0.32	C4H4O4	MALEIC ACID
720	S-PENTANOLS	195		-0.32	-0.67	C4H4O4	MALEIC ACID
721	OCTANOL	255		1.81	1.81 =	C4H4S1	THIOPHENE
722	DIETHYL ETHER	212		0.46	0.52 A	C4H5BR1O4	BROMOSUCCINIC ACID
723	DIETHYL ETHER	46		0.84	0.86 A	C4H5BR1O4	BROMOSUCCINIC ACID
724	1-BUTANOL	4		0.75	0.55	C4H5BR1O4	BROMOSUCCINIC ACID
725	XYLENE	46		-1.44	0.22 A	C4H5BR1O4	BROMOSUCCINIC ACID
726	OCTANOL	218		1.18	1.18 =	C4H5F3O2	ACETIC ACID, TRIFLUORO-ETHYL ESTER
727	OCTANOL	186		0.75	0.75 =	C4H5N1	PYRROLE
728	DIETHYL ETHER	3		-1.51	-1.21 A	C4H5N1O2	SUCCINIMIDE
729	DIETHYL ETHER	113		-1.42	-1.13 A	C4H5N1O2	SUCCINIMIDE
730	CHCL3	113		-1.27	-0.58	C4H5N1O2	SUCCINIMIDE
731	OILS	2		-2.31	-0.91 A	C4H5N1O2	SUCCINIMIDE
732	OILS	173		2.02	2.11 B	C4H5N1S1	ISOTHIOCYANATE,ALLYL
733	OCTANOL	218		-0.22	-0.22 =	C4H5N3	PYRIMIDINE,2-AMINO
734	N-BUTANOL	253	36	-0.68	-1.46	C4H5N3O1	CYTOSINE
735	OCTANE	256		-1.47		C4H5N3O2	2-METHYL-5-NITROIMIDAZOLE
736	OCTANE	256		-1.60		C4H5N3O2	4-METHYL-5-NITROIMIDAZOLE
737	N-BUTANOL	253	36	-1.54	-2.65	C4H5N3O3	URAMIL
738	OCTANOL	134		0.38	0.38 =	C4H6N4O1S1	3-METHYLTHIO-4-AMINO-1,2,4-TRIAZINE-5-ONE
739	OCTANOL	217	07	-0.25	-0.25 =	C4H6N4O3S2	2-ACETYLAMINO-1,3,4-THIADIAZOLE-5-SULFONAMIDE
740	CHCL3	217	07	-2.39		C4H6N4O3S2	2-ACETYLAMINO-1,3,4-THIADIAZOLE-5-SULFONAMIDE
741	OCTANOL	218		-0.26	-0.26 =	C4H6N4O3S2	1,3,4-THIADIAZOLE-2-SULFONAMIDE,5-ACETAMIDO
742	OILS	240		2.51	2.76 B	C4H6N4O12	ERYTHRITOL TETRANITRATE
743	OILS	257	12	1.66	1.81 B	C4H6O1	DIVINYL ETHER
744	OILS	258		0.40	0.77 B	C4H6O1	DIVINYL ETHER
745	OILS	259		1.61	1.77 B	C4H6O1	DIVINYL ETHER
746	OCTANOL	260		0.60	0.60 =	C4H6O1S1	G-THIOBUTYROLACTONE
747	OCTANOL	261		0.72	0.72 =	C4H6O2	CROTONIC ACID
748	DIETHYL ETHER	192		0.72	0.74 A	C4H6O2	CROTONIC ACID
749	DIETHYL ETHER	46		0.55	0.61 A	C4H6O2	CROTONIC ACID
750	CHCL3	29		-0.50	0.76 A	C4H6O2	CROTONIC ACID
751	CHCL3	46		-0.56	0.71 A	C4H6O2	CROTONIC ACID
752	BENZENE	29		-0.91	0.48 A	C4H6O2	CROTONIC ACID
753	XYLENE	46		-1.05	0.64 A	C4H6O2	CROTONIC ACID
754	TOLUENE	29		-1.05	0.64 A	C4H6O2	CROTONIC ACID
755	OCTANOL	5		-0.59	-0.59 =	C4H6O4	SUCCINIC ACID
756	DIETHYL ETHER	212		-0.87	-0.64 A	C4H6O4	SUCCINIC ACID
757	DIETHYL ETHER	3		-0.82	-0.60 A	C4H6O4	SUCCINIC ACID
758	DIETHYL ETHER	192		-0.89	-0.66 A	C4H6O4	SUCCINIC ACID
759	DIETHYL ETHER	194		-0.90	-0.67 A	C4H6O4	SUCCINIC ACID
760	DIETHYL ETHER	46		-0.65	-0.45 A	C4H6O4	SUCCINIC ACID
761	DIETHYL ETHER	62		-0.83	-0.61 A	C4H6O4	SUCCINIC ACID
762	DIETHYL ETHER	213		-0.84	-0.62 A	C4H6O4	SUCCINIC ACID
763	DIETHYL ETHER	36		-0.86	-0.63 A	C4H6O4	SUCCINIC ACID
764	CHCL3	46		-1.92	-0.53 A	C4H6O4	SUCCINIC ACID
765	N-BUTANOL	194		0.00	-0.51	C4H6O4	SUCCINIC ACID
766	1-BUTANOL	4		-0.02	-0.53	C4H6O4	SUCCINIC ACID
767	PRIM. PENTANOLS	182		-0.15	-0.59	C4H6O4	SUCCINIC ACID
768	PRIM. PENTANOLS	48		-0.19	-0.54	C4H6O4	SUCCINIC ACID
769	ETHYL ACETATE	194		-0.63	-0.77	C4H6O4	SUCCINIC ACID
770	CYCLOHEXANONE	194		0.04	-0.80	C4H6O4	SUCCINIC ACID
771	HEXANOL	74		-0.34		C4H6O4	SUCCINIC ACID
772	2-BUTANONE	194		0.00	-0.68	C4H6O4	SUCCINIC ACID
773	ME-I-BUT.KETONE	194		-0.73	-2.14	C4H6O4	SUCCINIC ACID
774	ME-I-BUT.KETONE	195		-0.69	-0.69	C4H6O4	SUCCINIC ACID
775	S-PENTANOLS	195		-0.23	-0.57	C4H6O4	SUCCINIC ACID
776	DIETHYL ETHER	3		-1.52	-1.22 A	C4H6O5	DIGLYCOLIC ACID
777	DIETHYL ETHER	207		-1.54	-1.24 A	C4H6O5	DIGLYCOLIC ACID
778	1-BUTANOL	4		-0.31	-0.94	C4H6O5	DIGLYCOLIC ACID
779	ME-I-BUT.KETONE	195		-1.27	-1.18	C4H6O5	DIGLYCOLIC ACID
780	S-PENTANOLS	195		-0.62	-1.02	C4H6O5	DIGLYCOLIC ACID
781	OCTANOL	5		-1.26	-1.26 =	C4H6O5	MALIC ACID
782	DIETHYL ETHER	207		-1.88	-1.53 A	C4H6O5	MALIC ACID
783	DIETHYL ETHER	213		-1.85	-1.49 A	C4H6O5	MALIC ACID
784	1-BUTANOL	4		-0.63	-1.39	C4H6O5	MALIC ACID
785	OLEYL ALCOHOL	5		-1.74	-1.16	C4H6O5	MALIC ACID
786	S-PENTANOLS	195		-0.97	-1.42	C4H6O5	MALIC ACID
787	ME-I-BUT.KETONE	195		-1.36	-1.27	C4H6O5	D-L-MALIC ACID
788	DIETHYL ETHER	192		-2.43	-2.02 A	C4H6O6	TARTARIC ACID
789	DIETHYL ETHER	46	12	-1.01	-0.76 A	C4H6O6	TARTARIC ACID
790	DIETHYL ETHER	213		-2.42	-2.01 A	C4H6O6	TARTARIC ACID
791	DIETHYL ETHER	36		-2.34	-1.93 A	C4H6O6	TARTARIC ACID
792	1-BUTANOL	4		-0.78	-1.60	C4H6O6	TARTARIC ACID
793	PRIM. PENTANOLS	48		-1.21	-1.84	C4H6O6	TARTARIC ACID
794	S-PENTANOLS	195		-1.10	-1.56	C4H6O6	TARTARIC ACID
795	ME-I-BUT.KETONE	195		-1.58	-1.47	C4H6O6	D-TARTARIC ACID
796	OILS	173		1.12	1.35 B	C4H7BR1O2	BROMOACETIC ACID, ETHYL ESTER
797	OCTANOL	5		1.42	1.42 =	C4H7BR1O2	A-BROMOBUTYRIC ACID
798	CHCL3	29		0.08	1.29 A	C4H7BR1O2	A-BROMOBUTYRIC ACID
799	OILS	209		0.14	1.12 A	C4H7BR1O2	A-BROMOBUTYRIC ACID
800	BENZENE	29		-0.08	1.33 A	C4H7BR1O2	A-BROMOBUTYRIC ACID

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801	I-BUTANOL	4		1.46	1.55	C4H7BR1O2	A-BROMOBUTYRIC ACID
802	TOLUENE	29		-0.27	1.32 A	C4H7BR1O2	A-BROMOBUTYRIC ACID
803	OCTANOL	262		1.40	1.40 =	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
804	DIETHYL ETHER	262		1.36	2.06	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
805	CYCLOHEXANE	262		0.55		C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
806	CHCL3	262		1.43	1.93 N	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
807	BENZENE	262		1.46	1.56 B	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
808	N-BUTANOL	262		1.65	1.83	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
809	ETHYL ACETATE	262		1.48	1.53	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
810	N-BUTYL ACETATE	262		1.48	1.52	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
811	CCL4	262		0.92	2.06 N	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
812	N-HEPTANE	262		0.36		C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
813	2-BUTANONE	262		0.72	0.81	C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
814	OCTANE	262		0.30		C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
815	CS2	262		0.71		C4H7CL2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL
816	OCTANOL	218		2.03	2.03 =	C4H7CL3O1	B,B,B-TRICHLORO-T-BUTANOL
817	OILS	224		1.36	2.44 A	C4H7CL3O1	B,B,B-TRICHLORO-T-BUTANOL
818	OILS	214		0.20	1.37 A	C4H7CL3O2	A,A,B-TRICL-N-BUTYRALDEHYDE HYDRATE
819	OILS	173		1.53	1.68 B	C4H7I1O2	IODOACETIC ACID, ETHYL ESTER
820	DIETHYL ETHER	112		1.23	1.21 A	C4H7N1O2	DIACETYLMONOXIME
821	CHCL3	112		0.08	0.65 N	C4H7N1O2	DIACETYLMONOXIME
822	PRIM. PENTANOLS	263		2.38	2.70	C4H7N1O2	DIACETYLMONOXIME
823	DIETHYL ETHER	207		-2.18	-1.80 A	C4H7N1O3	ACETIC ACID, ACETYLAMINO/ACETYL GLYCINE/
824	CHCL3	67		-2.78		C4H7N1O3	ACETIC ACID, ACETYLAMINO/ACETYL GLYCINE/
825	ETHYL ACETATE	67	12	-1.56	-1.73	C4H7N1O3	ACETIC ACID, ACETYLAMINO/ACETYL GLYCINE/
826	ME-1-BUT.KETONE	195		-1.50	-1.40	C4H7N1O3	ACETIC ACID,ACETYLAMINO/ACETYL GLYCINE/
827	S-PENTANOLS	195		-0.88	-1.31	C4H7N1O3	ACETIC ACID,ACETYLAMINO/ACETYL GLYCINE/
828	OCTANOL	260		-0.05	-0.05 =	C4H7N1S1	2-AZACYCLOPENTANTHIONE
829	N-BUTANOL	253	36	-0.31	-0.95	C4H7N5	4,5,6-TRIAMINOPYRIMIDINE
830	OCTANOL	56		-3.20	-3.20 =	C4H7NA1O2	BUTYRIC ACID, SODIUM SALT
831	OILS	264	12	-0.15	1.05 A	C4H8BR1N1O1	A-BROMO-I-BUTYRAMIDE
832	OCTANOL	238		0.34	0.34 =	C4H8BR1N1O1	BROMOACETAMIDE,N-ETHYL
833	OCTANOL	262		0.51	0.51 =	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
834	DIETHYL ETHER	262		-0.29	0.59 B	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
835	CYCLOHEXANE	262		-1.70		C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
836	CHCL3	262		-0.10	0.51 N	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
837	BENZENE	262		-0.82	0.57 A	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
838	N-BUTANOL	262		0.93	0.81	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
839	ETHYL ACETATE	262		0.40	0.37	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
840	N-BUTYL ACETATE	262		0.45	0.85	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
841	CCL4	262		-1.40	0.67 A	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
842	N-HEPTANE	262		-2.00		C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
843	2-BUTANONE	262		0.08	-0.52	C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
844	OCTANE	262		-2.00		C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
845	CS2	262		-1.70		C4H8CL3O4P1	DIME-1-OH-2,2,2-TRICLETHYL PHOSPHONATE/DIPTEREX/
846	OCTANOL	238		0.52	0.52 =	C4H8N2	2-IMIDAZOLINE,2-METHYL
847	CHCL3	265		-0.95	-0.29 N	C4H8N2O2	DIMETHYLGLYOXIME
848	N-BUTANOL	266		-1.08	-2.16	C4H8N2O2	DIMETHYLGLYOXIME
849	N-BUTANOL	253	36	-1.32	-2.35	C4H8N6	TETRAMINOPYRIMIDINE
850	OILS	267		0.61	0.94 B	C4H8O1	ALLYL METHYL ETHER
851	OCTANOL	186		0.29	0.29 =	C4H8O1	2-BUTANONE
852	OCTANOL	5		0.26	0.26 =	C4H8O1	2-BUTANONE
853	1-BUTANOL	4		1.20	1.18	C4H8O1	BUTYRALDEHYDE
854	OILS	259		0.83	1.20 B	C4H8O1	CYCLOPROPYL METHYL ETHER
855	OILS	267		0.70	1.02 B	C4H8O1	CYCLOPROPYL METHYL ETHER
856	OCTANOL	268		1.04	1.04 =	C4H8O1	ETHYL VINYL ETHER
857	OILS	258		-0.30	0.19 B	C4H8O1	ETHYL VINYL ETHER
858	OCTANOL	186		0.73	0.73 =	C4H8O2	ACETIC ACID, ETHYL ESTER
859	OCTANOL	5		0.66	0.66 =	C4H8O2	ACETIC ACID, ETHYL ESTER
860	DIETHYL ETHER	3	50	0.93	0.93 A	C4H8O2	ACETIC ACID,ETHYL ESTER
861	OILS	2		0.40	0.79 B	C4H8O2	ACETIC ACID,ETHYL ESTER
862	OILS	224		0.60	0.94 B	C4H8O2	ACETIC ACID,ETHYL ESTER
863	BENZENE	245	12	1.01	1.25 B	C4H8O2	ACETIC ACID,ETHYL ESTER
864	I-BUTANOL	4		0.86	0.70	C4H8O2	ACETIC ACID,ETHYL ESTER
865	CCL4	245		0.95	2.68 A	C4H8O2	ACETIC ACID,ETHYL ESTER
866	CS2	245		0.72		C4H8O2	ACETIC ACID,ETHYL ESTER
867	OCTANOL	5		0.79	0.79 =	C4H8O2	BUTYRIC ACID
868	DIETHYL ETHER	190		0.66	0.69 A	C4H8O2	BUTYRIC ACID
869	DIETHYL ETHER	207		0.68	0.71 A	C4H8O2	BUTYRIC ACID
870	DIETHYL ETHER	46		0.66	0.69 A	C4H8O2	BUTYRIC ACID
871	DIETHYL ETHER	49		0.81	0.82 A	C4H8O2	BUTYRIC ACID
872	CHCL3	29		-0.27	0.97 A	C4H8O2	BUTYRIC ACID
873	CHCL3	46		-0.27	0.97 A	C4H8O2	BUTYRIC ACID
874	OILS	209		-0.21	1.05 A	C4H8O2	BUTYRIC ACID
875	OILS	220		-0.35	0.87 A	C4H8O2	BUTYRIC ACID
876	OILS	193		-0.46	0.82 A	C4H8O2	BUTYRIC ACID
877	BENZENE	44		-0.65	0.74 A	C4H8O2	BUTYRIC ACID
878	BENZENE	29		-0.65	0.73 A	C4H8O2	BUTYRIC ACID
879	N-BUTANOL	190		0.95	0.85	C4H8O2	BUTYRIC ACID
880	I-BUTANOL	4		0.97	0.86	C4H8O2	BUTYRIC ACID
881	I-BUTANOL	184		0.96	0.85	C4H8O2	BUTYRIC ACID
882	I-BUTANOL	48		0.91	0.78	C4H8O2	BUTYRIC ACID
883	SEC-BUTANOL	190		0.72	0.48	C4H8O2	BUTYRIC ACID
884	XYLENE	46		-0.78	0.93 A	C4H8O2	BUTYRIC ACID
885	TOLUENE	29		-0.82	0.84 A	C4H8O2	BUTYRIC ACID
886	NITROBENZENE	48		-0.42	0.50	C4H8O2	BUTYRIC ACID
887	PRIM. PENTANOLS	190		1.05	0.95	C4H8O2	BUTYRIC ACID
888	PRIM. PENTANOLS	184		0.97	0.93	C4H8O2	BUTYRIC ACID
889	PRIM. PENTANOLS	48		1.03	1.00	C4H8O2	BUTYRIC ACID
890	ETHYL ACETATE	194		0.72	0.72	C4H8O2	BUTYRIC ACID
891	CCL4	48		-1.02	0.99 A	C4H8O2	BUTYRIC ACID
892	DI-I-PR. ETHER	221		0.24	0.83 A	C4H8O2	BUTYRIC ACID
893	2-BUTANONE	190		0.70	0.78	C4H8O2	BUTYRIC ACID
894	OCTANE	60	47	-1.76		C4H8O2	BUTYRIC ACID
895	OLEYL ALCOHOL	5		0.46	1.02	C4H8O2	BUTYRIC ACID
896	O-NITROTOLUENE	48		-0.44		C4H8O2	BUTYRIC ACID
897	S-PENTANOLS	190		1.01	0.86	C4H8O2	BUTYRIC ACID
898	PARAFFINS	197		-1.15		C4H8O2	BUTYRIC ACID
899	DODECANE	60	47	-1.87		C4H8O2	BUTYRIC ACID
900	HEXADECANE	60	47	-1.92		C4H8O2	BUTYRIC ACID

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
901	CHCL3	51		-0.25	1.00 A	C4H8O2	I-BUTYRIC ACID
902	CHCL3	29		-0.28	0.96 A	C4H8O2	I-BUTYRIC ACID
903	OILS	209		-0.12	1.13 A	C4H8O2	I-BUTYRIC ACID
904	BENZENE	51		-0.74	0.69 A	C4H8O2	I-BUTYRIC ACID
905	BENZENE	29		-0.72	0.71 A	C4H8O2	I-BUTYRIC ACID
906	BENZENE	46		-0.81	0.58 A	C4H8O2	I-BUTYRIC ACID
907	XYLENE	46		-0.80	0.91 A	C4H8O2	I-BUTYRIC ACID
908	TOLUENE	51		-0.86	0.88 A	C4H8O2	I-BUTYRIC ACID
909	TOLUENE	29		-0.87	0.82 A	C4H8O2	I-BUTYRIC ACID
910	NITROBENZENE	48		-0.42	0.50	C4H8O2	I-BUTYRIC ACID
911	PRIM. PENTANOLS	48		0.99	0.95	C4H8O2	I-BUTYRIC ACID
912	CCL4	37		-1.47	0.61 A	C4H8O2	I-BUTYRIC ACID
913	OCTANOL	5		-0.42	-0.42 =	C4H8O2	DIOXANE
914	CCL4	234	12	-0.13		C4H8O2	DIOXANE
915	OCTANOL	56		0.83	0.83 =	C4H8O2	FORMIC ACID, PROPYL ESTER
916	DIETHYL ETHER	46		-0.40	-0.23 A	C4H8O3	BUTYRIC ACID,B-HYDROXY
917	DIETHYL ETHER	207		-0.34	-0.18 A	C4H8O3	ETHOXYACETIC ACID
918	OCTANOL	5		-0.36	-0.36 =	C4H8O3	A-HYDROXY-1-BUTYRIC ACID
919	DIETHYL ETHER	192		-0.65	-0.45 A	C4H8O3	A-HYDROXY-I-BUTYRIC ACID
920	I-BUTANOL	4		0.08	-0.38	C4H8O3	A-HYDROXY-I-BUTYRIC ACID
921	OLEYL ALCOHOL	5		-0.85	-0.28	C4H8O3	A-HYDROXY-I-BUTYRIC ACID
922	DIETHYL ETHER	269		-0.48	-0.31 A	C4H8O3	A-HYDROXYBUTYRIC ACID
923	DIETHYL ETHER	46		-0.08	0.19 A	C4H8O3	A-HYDROXYBUTYRIC ACID
924	PRIM. PENTANOLS	269		0.05	-0.32	C4H8O3	A-HYDROXYBUTYRIC ACID
925	DIETHYL ETHER	3		-0.43	-0.26 A	C4H8O3	LACTIC ACID,METHYL ESTER
926	OCTANOL	186		2.39	2.39 =	C4H9CL1	I-CHLOROBUTANE
927	OCTANOL	186		-0.21	-0.21 =	C4H9N1O1	BUTYRAMIDE
928	DIETHYL ETHER	3		-1.24	-0.24 B	C4H9N1O1	BUTYRAMIDE
929	OILS	2		-2.02	-0.65 A	C4H9N1O1	BUTYRAMIDE
930	1-BUTANOL	4		0.18	-0.25	C4H9N1O1	BUTYRAMIDE
931	OCTANOL	235		-0.77	-0.77 =	C4H9N1O1	N,N-DIMETHYLACETAMIDE
932	OCTANOL	218		-1.08	-1.08 =	C4H9N1O1	MORPHOLINE
933	DIETHYL ETHER	3	12	-5.58	-4.76 A	C4H9N1O2	A-AMINOBUTYRIC ACID
934	N-BUTANOL	225		-1.34	-2.38	C4H9N1O2	A-AMINOBUTYRIC ACID
935	I-BUTANOL	4		-1.79	-3.02	C4H9N1O2	A-AMINOBUTYRIC ACID
936	SEC-BUTANOL	84	19	-0.79	-1.61	C4H9N1O2	A-AMINOBUTYRIC ACID
937	OCTANOL	65		1.01	1.01 =	C4H9N1O2	2-METHYL-2-NITROPROPANE
938	OCTANOL	270		1.17		C4H9N1O2	2-METHYL-2-NITROPROPANE
939	OCTANOL	235		2.15	2.15 =	C4H9N1O3	BUTYL NITRATE
940	OILS	271		0.43	0.81 B	C4H10F1O3P1	DIETHYLFLUOROPHOSPHATE
941	CCL4	228		0.54	0.44 B	C4H10F1O3P1	DIETHYLFLUOROPHOSPHATE
942	CCL4	271		0.54	0.44 B	C4H10F1O3P1	DIETHYLFLUOROPHOSPHATE
943	OCTANOL	5		-1.17	-1.17 =	C4H10N2	PIPERAZINE
944	DIETHYL ETHER	3	12	-3.28	-2.03 B	C4H10N2	PIPERAZINE
945	1-BUTANOL	4		-0.60	-1.36	C4H10N2	PIPERAZINE
946	DIETHYL ETHER	198		-0.41	-0.24 A	C4H10N2S1	PROPYLTHIOUREA
947	OCTANOL	216		0.88	0.88 =	C4H10O1	BUTANOL
948	DIETHYL ETHER	3		0.89	0.89 A	C4H10O1	BUTANOL
949	DIETHYL ETHER	174		0.57	0.63 A	C4H10O1	BUTANOL
950	CYCLOHEXANE	272		-0.72		C4H10O1	BUTANOL
951	CYCLOHEXANE	82		-1.12		C4H10O1	BUTANOL
952	CHCL3	174		0.45	1.03 N	C4H10O1	BUTANOL
953	OILS	173		-0.28	0.94 A	C4H10O1	BUTANOL
954	OILS	201		-0.20	1.02 A	C4H10O1	BUTANOL
955	BENZENE	272		-0.19	1.19 A	C4H10O1	BUTANOL
956	BENZENE	82		-0.34	0.96 A	C4H10O1	BUTANOL
957	BENZENE	231		-0.38	1.00	C4H10O1	BUTANOL
958	CCL4	272		-0.44		C4H10O1	BUTANOL
959	HEXANE	82		-0.78		C4H10O1	BUTANOL
960	OCTANE	59		-0.81		C4H10O1	BUTANOL
961	OLEYL ALCOHOL	82	12	-0.19	0.38	C4H10O1	BUTANOL
962	DODECANE	59		-0.96		C4H10O1	BUTANOL
963	HEXADECANE	59		-1.08		C4H10O1	BUTANOL
964	OCTANOL	5		0.83	0.83 =	C4H10O1	I-BUTANOL
965	OCTANOL	216		0.65	0.65 =	C4H10O1	I-BUTANOL
966	DIETHYL ETHER	3		0.84	0.85 A	C4H10O1	I-BUTANOL
967	DIETHYL ETHER	174		0.53	0.59 A	C4H10O1	I-BUTANOL
968	CHCL3	174		0.34	0.92 N	C4H10O1	I-BUTANOL
969	OILS	173		-0.36	0.86 A	C4H10O1	I-BUTANOL
970	OILS	101		-0.24	0.97 A	C4H10O1	I-BUTANOL
971	OILS	201		-0.26	0.96 A	C4H10O1	I-BUTANOL
972	I-BUTANOL	4		0.93	0.80	C4H10O1	I-BUTANOL
973	OCTANOL	186		0.61	0.61 =	C4H10O1	S-BUTANOL
974	DIETHYL ETHER	3		0.65	0.68 A	C4H10O1	S-BUTANOL
975	DIETHYL ETHER	174		0.28	0.12 A	C4H10O1	S-BUTANOL
976	CHCL3	174		0.30	0.89 N	C4H10O1	S-BUTANOL
977	OILS	2		-0.60	0.65 A	C4H10O1	S-BUTANOL
978	OILS	201		-0.42	0.81 A	C4H10O1	S-BUTANOL
979	OCTANOL	186		0.37	0.37 =	C4H10O1	T-BUTANOL
980	DIETHYL ETHER	3		0.34	0.41 A	C4H10O1	T-BUTANOL
981	DIETHYL ETHER	174		-0.08	0.06 A	C4H10O1	T-BUTANOL
982	CHCL3	174		-0.04	0.57 N	C4H10O1	T-BUTANOL
983	OILS	173		-0.64	0.61 A	C4H10O1	T-BUTANOL
984	OILS	224		-0.74	0.52 A	C4H10O1	T-BUTANOL
985	OILS	201		-0.66	0.59 A	C4H10O1	T-BUTANOL
986	OCTANOL	218		0.77	0.77 =	C4H10O1	ETHYL ETHER
987	OCTANOL	5		0.83	0.83 =	C4H10O1	ETHYL ETHER
988	DIETHYL ETHER	3	50	1.00	0.99 A	C4H10O1	ETHYL ETHER
989	OILS	173		0.58	0.93 B	C4H10O1	ETHYL ETHER
990	OILS	82		0.38	0.78 B	C4H10O1	ETHYL ETHER
991	OILS	258		0.36	0.74 B	C4H10O1	ETHYL ETHER
992	OILS	259		0.60	0.93 B	C4H10O1	ETHYL ETHER
993	DIETHYL ETHER	2		-1.38	-1.10 A	C4H10O2	1,3-BUTANEDIOL
994	OILS	2		-2.37	-0.93 A	C4H10O2	1,3-BUTANEDIOL
995	DIETHYL ETHER	2		-1.72	-1.38 A	C4H10O2	1,4-BUTANEDIOL
996	OILS	2		-2.68	-1.22 A	C4H10O2	1,4-BUTANEDIOL
997	OCTANOL	5		-0.92	-0.92 =	C4H10O2	2,3-BUTANEDIOL
998	DIETHYL ETHER	3		-1.54	-1.25 A	C4H10O2	2,3-BUTANEDIOL
999	OILS	2		-2.47	-1.03 A	C4H10O2	2,3-BUTANEDIOL
1000	OCTANOL	5		-0.54	-0.54 =	C4H10O2	ETHOXYETHANOL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1001	DIETHYL ETHER	2		-0.70	-0.50 A	C4H10O2	ETHOXYETHANOL
1002	OILS	2		-1.72	-0.33 A	C4H10O2	ETHOXYETHANOL
1003	OILS	173	12	-1.15	0.15 A	C4H10O2	ETHOXYETHANOL
1004	DIETHYL ETHER	3	12	-2.36	-1.98 A	C4H10O3	DIETHYLENEGLYCOL
1005	OILS	2		-2.58	-1.12 A	C4H10O3	GLYCEROL MONOMETHYL ETHER
1006	DIETHYL ETHER	3		-1.72	-1.39 A	C4H10O3	GLYCEROL,MONOMETHYLETHER
1007	1-BUTANOL	4		-1.43	-2.53	C4H10O4	ERYTHRITOL
1008	OCTANOL	235		2.28	2.28 =	C4H10S1	BUTANETHIOL
1009	OCTANOL	186		1.95	1.95 =	C4H10S1	DIETHYLSULFIDE
1010	OCTANOL	251		0.88	0.88 =	C4H11N1	BUTYLAMINE
1011	OCTANOL	218		0.81	0.81 =	C4H11N1	BUTYLAMINE
1012	OCTANOL	5		0.68	0.68 =	C4H11N1	BUTYLAMINE
1013	DIETHYL ETHER	251		0.11	0.94 B	C4H11N1	BUTYLAMINE
1014	CYCLOHEXANE	251		-0.29		C4H11N1	BUTYLAMINE
1015	CHCL3	251		0.99	0.62 B	C4H11N1	BUTYLAMINE
1016	BENZENE	251		0.14	0.65 B	C4H11N1	BUTYLAMINE
1017	1-BUTANOL	4		0.92	0.79	C4H11N1	BUTYLAMINE
1018	XYLENE	46		0.04	0.64 B	C4H11N1	BUTYLAMINE
1019	TOLUENE	150		0.30	1.84 A	C4H11N1	BUTYLAMINE
1020	CCL4	251		0.11	0.93 N	C4H11N1	BUTYLAMINE
1021	DI-I-PR. ETHER	251		-0.04	0.50	C4H11N1	BUTYLAMINE
1022	XYLENE	46		0.10	0.70 B	C4H11N1	I-BUTYLAMINE
1023	OCTANOL	218		0.40	0.40 =	C4H11N1	T-BUTYLAMINE
1024	OCTANOL	251		0.57	0.57 =	C4H11N1	DIETHYLAMINE
1025	OCTANOL	5		0.43	0.43 =	C4H11N1	DIETHYLAMINE
1026	DIETHYL ETHER	3		-0.28	0.68 B	C4H11N1	DIETHYLAMINE
1027	DIETHYL ETHER	251		-0.07	0.80 B	C4H11N1	DIETHYLAMINE
1028	CYCLOHEXANE	251		-0.34		C4H11N1	DIETHYLAMINE
1029	CHCL3	251		0.81	0.46 B	C4H11N1	DIETHYLAMINE
1030	CHCL3	46		0.89	0.53 B	C4H11N1	DIETHYLAMINE
1031	BENZENE	205		-0.02	0.54 B	C4H11N1	DIETHYLAMINE
1032	BENZENE	251		-0.05	0.52 B	C4H11N1	DIETHYLAMINE
1033	BENZENE	46		-0.05	0.52 B	C4H11N1	DIETHYLAMINE
1034	N-BUTANOL	37		0.43	0.08	C4H11N1	DIETHYLAMINE
1035	1-BUTANOL	4		0.74	0.53	C4H11N1	DIETHYLAMINE
1036	I-BUTANOL	37		0.42	0.07	C4H11N1	DIETHYLAMINE
1037	XYLENE	46		-0.10	0.50 B	C4H11N1	DIETHYLAMINE
1038	TOLUENE	205		-0.09	0.59 B	C4H11N1	DIETHYLAMINE
1039	TOLUENE	68		-0.20	0.51 B	C4H11N1	DIETHYLAMINE
1040	TOLUENE	273		-0.24	0.47 B	C4H11N1	DIETHYLAMINE
1041	PRIM. PENTANOLS	182		0.88	0.73	C4H11N1	DIETHYLAMINE
1042	CCL4	251		0.03	0.82 N	C4H11N1	DIETHYLAMINE
1043	CCL4	37		-0.10		C4H11N1	DIETHYLAMINE
1044	CLCH2CH2CL	37		-0.05		C4H11N1	DIETHYLAMINE
1045	DI-BUTYL ETHER	37		-0.20		C4H11N1	DIETHYLAMINE
1046	DI-I-PR. ETHER	251		-0.21	0.30	C4H11N1	DIETHYLAMINE
1047	OCTANOL	5		-1.43	-1.43 =	C4H11N1O2	DIETHANOLAMINE
1048	DIETHYL ETHER	3	50	-3.27	-2.02 B	C4H11N1O2	DIETHANOLAMINE
1049	1-BUTANOL	4		-0.70	-1.49	C4H11N1O2	DIETHANOLAMINE
1050	I-BUTANOL	184		-0.69	-1.48	C4H11N1O2	DIETHANOLAMINE
1051	CCL4	135		0.45	0.36 B	C4H11O2P1S2	PHOSPHORODITHIOTIC ACID,DIETHYL
1052	PRIM. PENTANOLS	236	17	0.46	0.28	C4H11O4P1	BUTYL PHOSPHATE
1053	DI-BUTYL ETHER	236	17	-0.18		C4H11O4P1	BUTYL PHOSPHATE
1054	DI-BUTYL ETHER	236	17	-0.27		C4H11O4P1	I-BUTYL PHOSPHATE
1055	CHCL3	274		-2.05	-0.65 A	C4H11O4P1	DIETHYL PHOSPHATE
1056	NITROBENZENE	274		-2.14	-0.90	C4H11O4P1	DIETHYL PHOSPHATE
1057	PRIM. PENTANOLS	236	17	0.23	0.00	C4H11O4P1	DIETHYL PHOSPHATE
1058	DI-I-PR. ETHER	274		-1.75	-1.50	C4H11O4P1	DIETHYL PHOSPHATE
1059	ME-I-BUT.KETONE	274		-0.56	-1.07	C4H11O4P1	DIETHYL PHOSPHATE
1060	S-PENTANOLS	274		0.35		C4H11O4P1	DIETHYL PHOSPHATE
1061	DIETHYL ETHER	3	12	-2.89	-1.69 B	C4H12N2	TETRAMETHYLENEDIAMINE
1062	1-BUTANOL	4		-0.12	-0.67	C4H12N2	TETRAMETHYLENEDIAMINE
1063	1-BUTANOL	184		-1.96		C4H13N1O1	TETRAMETHYLAMMONIUM HYDROXIDE
1064	OCTANOL	275	75	3.53	3.53 =	C5CL5N1	2,3,4,5,6 PENTACHLOROPYRIDINE (PKA= -1.00)
1065	OCTANOL	206	27	3.08	3.08 =	C5H1BR3N4	PURINE,2,6,8-TRIBROMO
1066	OCTANOL	206	27	3.90	3.90 =	C5H1CL3N4	PURINE,2,6,8,-TRICHLORO
1067	OCTANOL	275	75	3.32	3.32 =	C5H1CL4N1	2,3,5,6-TETRACHLOROPYRIDINE (PKA= -0.80)
1068	OCTANOL	275	75	2.68	2.68 =	C5H2CL3N1	2,4,6-TRICHLOROPYRIDINE (PKA= -0.30)
1069	OCTANOL	275	75	2.77	2.77 =	C5H2CL3N1	2,3,6-TRICHLOROPYRIDINE (PKA= -0.63)
1070	OCTANOL	275	75	3.11	3.11 =	C5H2CL3N1	2,3,5-TRICHLOROPYRIDINE (PKA= 0.78)
1071	OCTANOL	275	75	2.15	2.15 =	C5H3CL2N1	2,6-DICHLORPYRIDINE (PKA= 0.36)
1072	OCTANOL	275	75	2.40	2.40 =	C5H3CL2N1	2,5-DICHLORPYRIDINE (PKA= 2.62)
1073	OCTANOL	275	75	2.11	2.11 =	C5H3CL2N1	2,3-DICHLORPYRIDINE (PKA= 2.79)
1074	OCTANOL	275	75	2.56	2.56 =	C5H3CL2N1	3,5-DICHLORPYRIDINE (PKA= 3.20)
1075	OCTANOL	276		1.42	1.42 =	C5H4BR1N1	2-BROMOPYRIDINE
1076	OCTANOL	276		1.60	1.60 =	C5H4BR1N1	3-BROMOPYRIDINE /PKA= 2.84/
1077	OCTANOL	276		1.54	1.54 =	C5H4BR1N1	4-BROMOPYRIDINE
1078	OCTANOL	275	75	1.45	1.45 =	C5H4CL1N1	2-CHLOROPYRIDINE (PKA= 3.33)
1079	OCTANOL	275	75	1.43	1.43 =	C5H4CL1N1	3-CHLOROPYRIDINE (PKA= 4.28)
1080	OCTANOL	275	75	1.28	1.28 =	C5H4CL1N1	4-CHLOROPYRIDINE (PKA= 4.57)
1081	OCTANOL	276		1.27	1.27 =	C5H4CL1N1	2-CHLOROPYRIDINE
1082	OCTANOL	277	14	-1.11	-1.11 =	C5H4N4O1	HYPOXANTHINE
1083	N-BUTANOL	253	36	-0.27	-0.89	C5H4N4O1	HYPOXANTHINE
1084	N-BUTANOL	253	36	-0.34	-0.99	C5H4N4O2	XANTHINE
1085	OCTANOL	277	14	-2.92	-2.92 =	C5H4N4O3	URIC ACID
1086	N-BUTANOL	253	36	-0.96	-1.85	C5H4N4O3	URIC ACID
1087	OCTANOL	227		0.01	0.01 =	C5H4N4S1	MERCAPTOPURINE/PURINE-6-THIOL/(755)
1088	OCTANOL	227		0.01	0.01 =	C5H4N4S1	6-PURINETHIOL HYDRATE (NCS755)(PKA= 7.80)
1089	DIETHYL ETHER	192		0.55	0.60 A	C5H4O3	FURANE-2-CARBOXYLIC ACID
1090	DIETHYL ETHER	112		0.58	0.64 A	C5H4O3	FURANE-2-CARBOXYLIC ACID
1091	CHCL3	112		-0.54	0.73 A	C5H4O3	FURANE-2-CARBOXYLIC ACID
1092	CHCL3	278		0.30	1.55 A	C5H5F3O2	TRIFLUOROACETYLACETONE
1093	CHCL3	279		0.29	1.48 A	C5H5F3O2	TRIFLUOROACETYLACETONE
1094	BENZENE	279		0.11	1.52 A	C5H5F3O2	TRIFLUOROACETYLACETONE
1095	CCL4	279		-0.14	0.60 N	C5H5F3O2	TRIFLUOROACETYLACETONE
1096	HEXANE	279		-0.50		C5H5F3O2	TRIFLUOROACETYLACETONE
1097	O-DICL. BENZENE	279		-0.05		C5H5F3O2	TRIFLUOROACETYLACETONE
1098	OCTANOL	218		2.12	2.12 =	C5H5F5O2	PENTAFLUOROPROPIONIC ACID, ETHYL ESTER
1099	OCTANOL	276		0.64	0.64 =	C5H5N1	PYRIDINE /PKA = 5.23/
1100	OCTANOL	255		0.65	0.65 =	C5H5N1	PYRIDINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1101	DIETHYL ETHER	3		0.08	0.92 B	C5H5N1	PYRIDINE
1102	CHCL3	280		1.43	0.81 B	C5H5N1	PYRIDINE
1103	OILS	173		-0.02	0.42 B	C5H5N1	PYRIDINE
1104	BENZENE	183		0.42	0.84 B	C5H5N1	PYRIDINE
1105	BENZENE	281		0.39	0.82 B	C5H5N1	PYRIDINE
1106	BENZENE	66		0.44	0.85 B	C5H5N1	PYRIDINE
1107	1-BUTANOL	4		0.86	0.70	C5H5N1	PYRIDINE
1108	XYLENE	46		0.31	0.92 B	C5H5N1	PYRIDINE
1109	TOLUENE	188		0.16	0.77 B	C5H5N1	PYRIDINE
1110	OCTANOL	275	75	1.04	1.04 =	C5H5N1	PYRIDINE (PKA= 4.90)
1111	DIETHYL ETHER	248		-1.82	-0.75 B	C5H5N1O1	2-HYDROXYPYRIDINE
1112	CHCL3	248		-1.21	0.12 A	C5H5N1O1	2-HYDROXYPYRIDINE
1113	DIETHYL ETHER	248		-0.32	-0.16 A	C5H5N1O1	3-HYDROXYPYRIDINE
1114	CHCL3	248		-1.40	-0.06 A	C5H5N1O1	3-HYDROXYPYRIDINE
1115	OCTANOL	218		-1.69	-1.69 =	C5H5N1O1	PYRIDINE,1-OXIDE
1116	OCTANOL	277	14	-0.16	-0.16 =	C5H5N5	ADENINE
1117	N-BUTANOL	253	36	0.33	-0.07	C5H5N5	ADENINE
1118	N-BUTANOL	253	36	0.44	0.09	C5H5N5	ADENINE
1119	N-BUTANOL	253	36	-0.35	-1.00	C5H5N5O1	GUANINE
1120	N-BUTANOL	253	36	-0.55	-1.28	C5H5N5O1	ISOGUANINE
1121	N-BUTANOL	253	36	-0.32	-0.96	C5H5N5S1	2-THIOADENINE
1122	OCTANOL	227		-0.07	-0.07 =	C5H5N5S1	THIOGUANINE/2-AMINOPURINE-6-THIOL/(752)
1123	DIETHYL ETHER	3		-0.11	0.75 B	C5H6N2	2-AMINOPYRIDINE
1124	1-BUTANOL	4		0.65	0.41	C5H6N2	2-AMINOPYRIDINE
1125	OCTANOL	276		0.11	0.11 =	C5H6N2	3-AMINOPYRIDINE /PKA = 5.98/
1126	OCTANOL	276		0.28	0.28 =	C5H6N2	4-AMINOPYRIDINE /PKA = 9.17/
1127	CHCL3	282	12	-0.70	-0.97	C5H6N2	4-AMINOPYRIDINE
1128	OCTANOL	276		0.16	0.16 =	C5H6N2	4-METHYLPYRIMIDINE
1129	OCTANOL	235	70	0.22	0.22 =	C5H6N2O1S1	4-HYDROXY-2-METHYLTHIO-PYRIMIDINE/2-METHIOURACIL/
1130	OCTANOL	283		-1.20	-1.20 =	C5H6N2O2	1-METHYLURACIL
1131	N-BUTANOL	253	36	0.05	-0.44	C5H6N2O2	THYMINE
1132	DIETHYL ETHER	3		-0.62	-0.43 A	C5H6O4	CITRACONIC ACID
1133	DIETHYL ETHER	212		-0.45	-0.28 A	C5H6O4	ITACONIC ACID
1134	DIETHYL ETHER	207		-0.48	-0.31 A	C5H6O4	ITACONIC ACID
1135	I-BUTANOL	4		0.28	-0.11	C5H6O4	ITACONIC ACID
1136	ME-I-BUT.KETONE	195		-0.26	-0.30	C5H6O4	ITACONIC ACID
1137	OILS	284		-0.32	0.53 B	C5H7N3O1	3,5-DIMETHYL-4-NITROSOPYRAZOLE
1138	OCTANE	256		-0.39		C5H7N3O2	2-ETHYL-5-NITROIMIDAZOLE
1139	N-BUTANOL	253	36	-0.79	-1.61	C5H7N5O1	4,6-DIAMINO-5-FORMAMIDO-PYRIMIDINE
1140	N-BUTANOL	253	36	-0.02	-0.54	C5H7N5S1	4,6-DIAMINO-5-THIOFORMAMIDO-PYRIMIDINE
1141	OCTANOL	186		1.98	1.98 =	C5H8	1-PENTYNE
1142	OCTANOL	218		-0.68	-0.68 =	C5H8N2O3	UREA,1,3-DIACETYL
1143	OCTANOL	134		-0.16	-0.16 =	C5H8N4O1S1	3-METHIO-4-AMINO-6-ME-1,2,4-TRIAZINE-5-ONE
1144	OCTANOL	217		0.13	0.13 =	C5H8N4O3S2	2-ACETYLIMINO-3-ME-1,3,4-THIADIAZOLE-5-SULFONAMIDE
1145	CHCL3	217		-1.40		C5H8N4O3S2	2-ACETYLIMINO-3-ME-1,3,4-THIADIAZOLE-5-SULFONAMIDE
1146	OILS	259		1.83	1.95 B	C5H8O1	CYCLOPROPYL VINYL ETHER
1147	OILS	259		1.94	2.04 B	C5H8O1	I-PROPENYL VINYL ETHER
1148	CHCL3	285		0.77	1.90 A	C5H8O2	ACETYLACETONE
1149	BENZENE	286	4	0.76	2.14 A	C5H8O2	ACETYLACETONE
1150	BENZENE	287		0.90	2.25 A	C5H8O2	ACETYLACETONE
1151	DIETHYL ETHER	3		-0.58	-0.39 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1152	DIETHYL ETHER	207		-0.64	-0.45 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1153	DIETHYL ETHER	112		-0.64	-0.45 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1154	DIETHYL ETHER	46		-0.49	-0.31 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1155	CHCL3	112		-1.19	0.14 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1156	CHCL3	46		-1.32	0.02 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1157	I-BUTANOL	4		0.08	-0.39	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1158	XYLENE	46		-1.90	-0.27 A	C5H8O3	LEVULINIC ACID/B-ACETYLPROPIONIC ACID/
1159	DIETHYL ETHER	288		0.44	0.50 A	C5H8O4	DIMETHYLMALONIC ACID
1160	1-BUTANOL	4		0.69	0.46	C5H8O4	DIMETHYLMALONIC ACID
1161	PRIM. PENTANOLS	48		0.71	0.60	C5H8O4	DIMETHYLMALONIC ACID
1162	OLEYL ALCOHOL	5		-0.31	0.26	C5H8O4	DIMETHYLMALONIC ACID
1163	DIETHYL ETHER	212		-0.55	-0.37 A	C5H8O4	GLUTARIC ACID
1164	DIETHYL ETHER	207		-0.57	-0.39 A	C5H8O4	GLUTARIC ACID
1165	DIETHYL ETHER	194		-0.60	-0.40 A	C5H8O4	GLUTARIC ACID
1166	DIETHYL ETHER	46		-0.47	-0.29 A	C5H8O4	GLUTARIC ACID
1167	CHCL3	46		-1.81	-0.43 A	C5H8O4	GLUTARIC ACID
1168	N-BUTANOL	194		0.21	-0.25	C5H8O4	GLUTARIC ACID
1169	I-BUTANOL	4		0.30	-0.08	C5H8O4	GLUTARIC ACID
1170	ETHYL ACETATE	194		-0.18	-0.24	C5H8O4	GLUTARIC ACID
1171	ME-I-BUT.KETONE	195		-0.45	-0.47	C5H8O4	GLUTARIC ACID
1172	OLEYL ALCOHOL	5		-0.96	-0.39	C5H8O4	GLUTARIC ACID
1173	S-PENTANOLS	195		0.16	-0.13	C5H8O4	GLUTARIC ACID
1174	OILS	264		-0.03	1.16 A	C5H9BR1N2O2	A-BROMO-I-BUTYRYLUREA
1175	OILS	264		-0.43	0.80 A	C5H9BR1N2O2	A-BROMOBUTYRLUREA
1176	OILS	209		0.55	1.75 A	C5H9BR1O2	A-BROMOVALERIC ACID
1177	BENZENE	29		0.50	1.89 A	C5H9BR1O2	A-BROMOVALERIC ACID
1178	TOLUENE	29		0.38	1.88 A	C5H9BR1O2	A-BROMOVALERIC ACID
1179	OCTANOL	227		1.53	1.53 =	C5H9CL2N3O2	1,3-BIS(2-CHLOROETHYL)-I-NITROSOUREA (NCS 409962)
1180	DECANOL	289		1.39		C5H9CL2N3O2	1,3-BIS(2-CHLOROETHYL)-1-NITROSOUREA(409962)
1181	CHCL3	67		-2.20		C5H9N1O3	A-AMINOPROPIONIC ACID, N-ACETYL
1182	ETHYL ACETATE	67		-1.25	-1.40	C5H9N1O3	A-AMINOPROPIONIC ACID, N-ACETYL
1183	OILS	290		-0.87	0.40 A	C5H9N1O3	O-ETHYL CARBAMATE, N-ACETYL
1184	OCTANOL	260		0.13	0.13 =	C5H9N1S1	2-AZACYCLOHEXANTHIONE
1185	OCTANOL	255		2.03	2.03 =	C5H9N1S1	THIOCYANIC ACID,BUTYL ESTER
1186	OILS	239		1.99	2.10 B	C5H9N3O9	1,2,3-PENTANETRIOLTRINITRATE
1187	OILS	240		1.38	2.44 A	C5H9N3O10	PENTAERYTHRITOL TRINITRATE
1188	OILS	264		-0.20	1.00 A	C5H10BR1N1O1	A-BROMO-I-VALERAMIDE
1189	OILS	264		-0.62	0.63 A	C5H10BR1N1O1	A-BROMOVALERAMIDE
1190	PARAFFINS	241		-2.22		C5H10N2S1	IMIDAZOLIDONE,N-ETHYL-2-THIO/N-ETHYLETHYLENETHIOUREA
1191	OILS	258		0.30	0.69 B	C5H10O1	ALLYL ETHYL ETHER
1192	OILS	259		1.20	1.43 B	C5H10O1	CYCLOPROPYL ETHYL ETHER
1193	OILS	258		-0.21	0.26 B	C5H10O1	I-PROPENYL ETHYL ETHER
1194	BENZENE	245	12	1.52	1.60 B	C5H10O2	ACETIC ACID,PROPYL ESTER
1195	CCL4	245		1.59	1.39 B	C5H10O2	ACETIC ACID,PROPYL ESTER
1196	CS2	245		1.30		C5H10O2	ACETIC ACID,PROPYL ESTER
1197	DIETHYL ETHER	3		1.51	1.44 A	C5H10O2	ACETIC ACID,TRIMETHYL
1198	DIETHYL ETHER	207		1.11	1.09 A	C5H10O2	ACETIC ACID,TRIMETHYL
1199	I-BUTANOL	4		1.50	1.60	C5H10O2	ACETIC ACID,TRIMETHYL
1200	OCTANOL	186		1.21	1.21 =	C5H10O2	PROPIONIC ACID, ETHYL ESTER

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1201	DIETHYL ETHER	190		1.24	1.20 A	C5H10O2	VALERIC ACID
1202	DIETHYL ETHER	46		1.17	1.15 A	C5H10O2	VALERIC ACID
1203	DIETHYL ETHER	49		1.36	1.31 A	C5H10O2	VALERIC ACID
1204	CHCL3	29		0.34	1.53 A	C5H10O2	VALERIC ACID
1205	CHCL3	46		0.32	1.51 A	C5H10O2	VALERIC ACID
1206	OILS	209		0.48	1.69 A	C5H10O2	VALERIC ACID
1207	OILS	220		0.41	1.57 A	C5H10O2	VALERIC ACID
1208	BENZENE	44		-0.05	1.32 A	C5H10O2	VALERIC ACID
1209	BENZENE	29		-0.09	1.32 A	C5H10O2	VALERIC ACID
1210	N-BUTANOL	190		1.36	1.45	C5H10O2	VALERIC ACID
1211	I-BUTANOL	184		1.39	1.45	C5H10O2	VALERIC ACID
1212	SEC-BUTANOL	190		1.06	0.99	C5H10O2	VALERIC ACID
1213	XYLENE	46		-0.33	1.43 A	C5H10O2	VALERIC ACID
1214	TOLUENE	29		-0.20	1.37 A	C5H10O2	VALERIC ACID
1215	PRIM. PENTANOLS	190		1.55	1.60	C5H10O2	VALERIC ACID
1216	PRIM. PENTANOLS	184		1.40	1.50	C5H10O2	VALERIC ACID
1217	2-BUTANONE	190		1.01	1.40	C5H10O2	VALERIC ACID
1218	OCTANE	60	47	-1.18		C5H10O2	VALERIC ACID
1219	S-PENTANOLS	190		1.44	1.35	C5H10O2	VALERIC ACID
1220	PARAFFINS	291	12	-2.54		C5H10O2	VALERIC ACID
1221	DODECANE	60	47	-1.25		C5H10O2	VALERIC ACID
1222	HEXADECANE	60	47	-1.31		C5H10O2	VALERIC ACID
1223	CHCL3	48		0.21	1.40 A	C5H10O2	I-VALERIC ACID
1224	CHCL3	29		0.17	1.37 A	C5H10O2	I-VALERIC ACID
1225	OILS	209		0.27	1.51 A	C5H10O2	I-VALERIC ACID
1226	BENZENE	29		-0.23	1.19 A	C5H10O2	I-VALERIC ACID
1227	I-BUTANOL	4		1.30	1.32	C5H10O2	I-VALERIC ACID
1228	I-BUTANOL	48		1.13	1.08	C5H10O2	I-VALERIC ACID
1229	XYLENE	48		-0.31	1.48 A	C5H10O2	I-VALERIC ACID
1230	TOLUENE	29		-0.35	1.24 A	C5H10O2	I-VALERIC ACID
1231	NITROBENZENE	48		0.07	0.93	C5H10O2	I-VALERIC ACID
1232	PRIM. PENTANOLS	48		1.13	1.13	C5H10O2	I-VALERIC ACID
1233	CCL4	48		-0.54		C5H10O2	I-VALERIC ACID
1234	O-NITROTOLUENE	48		-0.05		C5H10O2	I-VALERIC ACID
1235	XYLENE	46		-0.10	1.67 A	C5H10O2	I-VALERIC AICD
1236	DIETHYL ETHER	3		-1.39	-1.10 A	C5H10O4	GLYCEROL MONOACETATE/MONACETIN/
1237	OILS	214	12	-1.22	0.10 A	C5H10O4	GLYCEROL MONOACETATE/MONACETIN/
1238	OILS	70		-1.18	0.14 A	C5H10O4	GLYCEROL MONOACETATE/MONACETIN/
1239	I-BUTANOL	4		-1.72	-2.92	C5H10O5	ARABINOSE
1240	OCTANOL	277	14	-2.32	-2.32 =	C5H10O5	RIBOSE
1241	OCTANOL	186		2.33	2.33 =	C5H11F1	1-FLUOROPENTANE
1242	OCTANOL	218		0.85	0.85 =	C5H11N1	PIPERIDINE
1243	DIETHYL ETHER	3		-0.24	0.64 B	C5H11N1	PIPERIDINE
1244	DIETHYL ETHER	46		-0.18	0.69 B	C5H11N1	PIPERIDINE
1245	CHCL3	46		0.92	0.56 B	C5H11N1	PIPERIDINE
1246	BENZENE	183		-0.06	0.51 B	C5H11N1	PIPERIDINE
1247	I-BUTANOL	4		0.78	0.59	C5H11N1	PIPERIDINE
1248	XYLENE	46		0.03	0.63 B	C5H11N1	PIPERIDINE
1249	CCL4	234	12	-0.82		C5H11N1O1	DIMETHYLPROPIONAMIDE
1250	OCTANOL	218		-0.33	-0.33 =	C5H11N1O1	MORPHOLINE,4-METHYL
1251	OILS	82		-1.15	0.19 A	C5H11N1O1	VALERAMIDE
1252	OILS	292	12	-0.50	0.73 A	C5H11N1O1	VALERAMIDE
1253	OLEYL ALCOHOL	82		-0.52	0.05	C5H11N1O1	VALERAMIDE
1254	DIETHYL ETHER	3		-0.77	0.17 B	C5H11N1O1	I-VALERAMIDE
1255	OILS	2		-1.64	-0.30 A	C5H11N1O1	I-VALERAMIDE
1256	N-BUTANOL	225		-0.98	-2.02	C5H11N1O2	A-AMINOVALERIC ACID/NORVALINE/
1257	SEC-BUTANOL	84	19	-0.54	-1.26	C5H11N1O2	A-AMINOVALERIC ACID/NORVALINE/
1258	OILS	293		0.73	1.85 A	C5H11N1O2	O-1-BUTYLCARBAMATE
1259	N-BUTANOL	225		-1.14	-2.10	C5H11N1O2	VALINE
1260	CCL4	294		0.00		C5H11N1S2	N,N-DIETHYLDITHIOCARBAMIC ACID
1261	N-BUTANOL	295	52	-0.47	-1.17	C5H12CL1N1O2	VALINE HYDROCHLORIDE
1262	N-BUTANOL	295	52	-0.40	-1.07	C5H12CL1N1O2S1	METHIONINE HYDROCHLORIDE
1263	OILS	2		-2.12	-0.70 A	C5H12N2O1	N,N-DIETHYLUREA
1264	DIETHYL ETHER	3		-1.72	-0.50 B	C5H12N2O1	DIETHYLUREA,UNSYM.
1265	SEC-BUTANOL	84	19	-1.70	-2.89	C5H12N2O2	ORNITHINE
1266	OCTANOL	216		1.40	1.40 =	C5H12O1	PENTANOL
1267	OILS	201		0.36	1.52 A	C5H12O1	PENTANOL
1268	BENZENE	231		0.19	1.56 A	C5H12O1	PENTANOL
1269	CCL4	234	12	0.36		C5H12O1	PENTANOL
1270	OCTANE	59		-0.19		C5H12O1	PENTANOL
1271	DODECANE	59		-0.31		C5H12O1	PENTANOL
1272	HEXADECANE	59		-0.39		C5H12O1	PENTANOL
1273	OCTANOL	216		1.16	1.16 =	C5H12O1	1-PENTANOL
1274	DIETHYL ETHER	3		1.28	1.24 A	C5H12O1	1-PENTANOL
1275	OILS	173		0.26	1.43 A	C5H12O1	1-PENTANOL
1276	OILS	101		0.33	1.52 A	C5H12O1	1-PENTANOL
1277	OILS	201		0.32	1.48 A	C5H12O1	1-PENTANOL
1278	OILS	201		0.17	1.34 A	C5H12O1	2-PENTANOL
1279	OILS	201		0.20	1.37 A	C5H12O1	3-PENTANOL
1280	OCTANOL	186		1.36	1.36 =	C5H12O1	1-PROPANOL,2,2-DIMETHYL
1281	OCTANOL	80		0.89	0.89 =	C5H12O1	2-PROPANOL,2-ETHYL/T-AMYL ALCOHOL/
1282	OILS	173		-0.21	1.05 A	C5H12O1	2-PROPANOL,2-ETHYL/T-AMYL ALCOHOL/
1283	OILS	224		0.00	1.22 A	C5H12O1	2-PROPANOL,2-ETHYL/T-AMYL ALCOHOL/
1284	OILS	296		0.15	1.33 A	C5H12O1	2-PROPANOL,2-ETHYL/T-AMYL ALCOHOL/
1285	OILS	201		-0.04	1.15 A	C5H12O1	2-PROPANOL,2-ETHYL/T-AMYL ALCOHOL/
1286	OCTANOL	218		0.84	0.84 =	C5H12O2	DIETHOXYMETHANE
1287	DIETHYL ETHER	2		-1.26	-0.99 A	C5H12O2	1,5-PENTANEDIOL
1288	OILS	2		-2.21	-0.78 A	C5H12O2	1,5-PENTANEDIOL
1289	DIETHYL ETHER	3		-1.43	-1.14 A	C5H12O3	DIETHYLENE GLYCOL MONOMETHYL ETHER
1290	OILS	2		-2.38	-0.93 A	C5H12O3	DIETHYLENE GLYCOL MONOMETHYL ETHER
1291	DIETHYL ETHER	3		-1.58	-1.27 A	C5H12O3	GLYCERYL-A-MONOETHYL ETHER
1292	OILS	2		-2.13	-0.71 A	C5H12O3	GLYCERYL-A-MONOETHYL ETHER
1293	I-BUTANOL	4		-0.85	-1.70	C5H12O4	PENTAERYTHRITOL
1294	XYLENE	46		0.44	1.05 B	C5H13N1	AMYLAMINE
1295	DIETHYL ETHER	3		0.30	1.13 B	C5H13N1	1-AMYLAMINE
1296	OCTANOL	218		1.33	1.33 =	C5H13N1	METHYLBUTYLAMINE
1297	DI-BUTYL ETHER	236	17	-0.14		C5H13O4P1	AMYL PHOSPHATE
1298	OCTANOL	297	46	-3.00	-3.00 =	C5H14I1N1	TRIMETHYL-ETHYL-AMMONIUM IODIDE
1299	DIETHYL ETHER	3	12	-2.56	-1.42 B	C5H14N2	PENTAMETHYLENEDIAMINE
1300	I-BUTANOL	4		0.16	-0.28	C5H14N2	PENTAMETHYLENEDIAMINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1301	OCTANOL	298		3.22	3.22 =	C5H14SI1	SILANE, OIMETHYL-PROPYL
1302	OCTANOL	56		2.22	2.22 =	C6F6	HEXAFLUOROBENZENE
1303	OCTANOL	206	27	4.17		C6H1CL4N3	4,5,6,7-TETRACHLOROBENZOTRIAZOLE
1304	HEXANE	299		0.18		C6H1CL4N3	4,5,6,7-TETRACHLOROBENZOTRIAZOLE
1305	OCTANOL	56	49	5.01	5.01 =	C6H1CL5O1	PENTACHLOROPHENOL
1306	HEXANE	299		2.15		C6H1CL5O1	PENTACHLOROPHENOL
1307	CYCLOHEXANE	300		-0.52		C6H1F5O1	PENTAFLUOROPHENOL
1308	HEXANE	299		-0.30		C6H1F5O1	PENTAFLUOROPHENOL
1309	OLEYL ALCOHOL	300		2.37	2.91	C6H1F5O1	PENTAFLUOROPHENOL
1310	OLEYL ALCOHOL	300		2.09	2.64	C6H2F4O1	TETRAFLUOROPHENOL
1311	OI-I-PR. KETONE	93	46	-1.48		C6H2K1N3O7	POTASSIUM PICRATE
1312	OI-I-PR. KETONE	93	46	-1.62		C6H2N3NA1O7	SOOIUM PICRATE
1313	HEXANE	299		-1.30		C6H3CL1N4O2	5-CHLORO-4-NITROBENZOTRIAZOLE
1314	OCTANOL	56		3.72	3.72 =	C6H3CL3O1	2,4,5-TRICHLOROPHENOL
1315	OCTANOL	9		3.06	3.06 =	C6H3CL3O1	2,4,6-TRICHLOROPHENOL
1316	OCTANOL	56		3.69	3.69 =	C6H3CL3O1	2,4,6-TRICHLOROPHENOL
1317	CYCLOHEXANE	300		-0.15		C6H3F3O1	TRIFLUOROPHENOL
1318	OLEYL ALCOHOL	300		1.98	2.53	C6H3F3O1	TRIFLUOROPHENOL
1319	CHCL3	47		1.20	2.31 A	C6H3N3O1	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1320	OCTANOL	218		2.03	2.03 =	C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1321	BENZENE	33	12	1.69	3.02 A	C6H3N3O7	2,4,6-TRINITROPHENOL /PICRIC ACIO/
1322	N-BUTANOL	253	36	0.96	0.82	C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1323	TOLUENE	42		0.88	2.35 A	C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1324	TOLUENE	36	12	1.71	3.08 A	C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1325	PRIM. PENTANOLS	182		1.85	2.01	C6H3N3O7	2,4,6-TRINITROPHENOL /PICRIC ACIO/
1326	S-PENTANOLS	195	12	0.82	0.63	C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1327	TETRALIN	246		2.04		C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1328	BROMOFORM	47		0.04		C6H3N3O7	2,4,6-TRINITROPHENOL/PICRIC ACIO/
1329	OCTANOL	10		2.64	2.64 =	C6H4BR1N1O2	BENZENE,3-BROMO-1-NITRO
1330	OLEYL ALCOHOL	124		2.01	2.56	C6H4BR2O1	2,4-OIBROMOPHENOL
1331	OCTANOL	10		2.39	2.39 =	C6H4CL1N1O2	BENZENE,4-CHLORO-1-NITRO
1332	OCTANOL	10		2.46	2.46 =	C6H4CL1N1O2	BENZENE,3-CHLORO-1-NITRO
1333	OCTANOL	301		2.24	2.24 =	C6H4CL1N1O2	BENZENE,2-CHLORO-1-NITRO
1334	OCTANOL	301		2.41	2.41 =	C6H4CL1N1O2	BENZENE,3-CHLORO-1-NITRO
1335	OCTANOL	301		2.41	2.41 =	C6H4CL1N1O2	BENZENE,4-CHLORO-1-NITRO
1336	OCTANOL	301		3.38	3.38 =	C6H4CL2	M-OICHLOROBENZENE
1337	OCTANOL	301		3.38	3.38 =	C6H4CL2	O-OICHLOROBENZENE
1338	OCTANOL	301		3.39	3.39 =	C6H4CL2	P-OICHLOROBENZENE
1339	OLEYL ALCOHOL	124		2.54	3.08	C6H4I2O1	2,4-OI-IOOOPHENOL
1340	OCTANOL	283	73	-0.84	-0.84 =	C6H4N1NA1O3	SOOIUM P-NITROPHENOXIOE
1341	OCTANOL	283	71	-1.31	-1.31 =	C6H4N1NA1O3	SOOIUM P-NITROPHENOXIOE (PKA = 7.15)
1342	OCTANOL	10		1.49	1.49 =	C6H4N2O4	M-OINITROBENZENE
1343	OCTANOL	301		1.49	1.49 =	C6H4N2O4	M-OINITROBENZENE
1344	OCTANOL	301		1.58	1.58 =	C6H4N2O4	O-OINITROBENZENE
1345	OCTANOL	10		1.46	1.46 =	C6H4N2O4	P-OINITROBENZENE
1346	OCTANOL	301		1.49	1.49 =	C6H4N2O4	P-OINITROBENZENE
1347	OCTANOL	218		1.51	1.51 =	C6H4N2O5	2,4-OINITROPHENOL
1348	OCTANOL	302		1.54	1.54 =	C6H4N2O5	2,4-OINITROPHENOL
1349	OILS	173	12	1.35	2.38 A	C6H4N2O5	2,4-OINITROPHENOL
1350	HEXANE	299		0.55		C6H4N2O5	2,4-OINITROPHENOL
1351	OCTANOL	186		1.75	1.75 =	C6H4N2O5	2,5-OINITROPHENOL
1352	OCTANOL	218		1.75	1.75 =	C6H4N2O5	2,5-OINITROPHENOL
1353	OCTANOL	186		1.25	1.25 =	C6H4N2O5	2,6-OINITROPHENOL
1354	OCTANOL	218		1.18	1.18 =	C6H4N2O5	2,6-OINITROPHENOL
1355	OCTANOL	218		2.32	2.32 =	C6H4N2O5	3,5-OINITROPHENOL
1356	OCTANOL	218		2.36	2.36 =	C6H4N2O5	3,5-OINITROPHENOL
1357	OCTANOL	218		-0.13	-0.13 =	C6H4N4	ISOPROPENYLAMINE, 1,1,3-TRICYANO
1358	OCTANOL	206	27	1.95		C6H4N4O2	5-NITROBENZTRIAZOLE
1359	HEXANE	299		-2.60		C6H4N4O2	5-NITROBENZTRIAZOLE
1360	OCTANOL	238		0.20	0.20 =	C6H4O2	QUINONE
1361	OIETHYL ETHER	3		-0.49	0.39 B	C6H4O2	QUINONE
1362	OIETHYL ETHER	303		-0.51	0.40 B	C6H4O2	QUINONE
1363	CYCLOHEXANE	304		-0.39		C6H4O2	QUINONE
1364	OILS	305		0.27	0.69 B	C6H4O2	QUINONE
1365	OCTANOL	10		2.99	2.99 =	C6H5BR1	BROMOBENZENE
1366	OCTANOL	10		2.63	2.63 =	C6H5BR1O1	M-BROMOPHENOL
1367	CYCLOHEXANE	124		-0.52		C6H5BR1O1	M-BROMOPHENOL
1368	METH. OECANOATE	124		2.12	2.59	C6H5BR1O1	M-BROMOPHENOL
1369	OLEYL ALCOHOL	124		2.02	2.57	C6H5BR1O1	M-BROMOPHENOL
1370	OCTANOL	10		2.35	2.35 =	C6H5BR1O1	O-BROMOPHENOL
1371	CYCLOHEXANE	124		0.26		C6H5BR1O1	O-BROMOPHENOL
1372	METH. OECANOATE	124		1.48	1.93	C6H5BR1O1	O-BROMOPHENOL
1373	OLEYL ALCOHOL	124		1.36	1.91	C6H5BR1O1	O-BROMOPHENOL
1374	OCTANOL	10		2.59	2.59 =	C6H5BR1O1	P-BROMOPHENOL
1375	CYCLOHEXANE	56		-0.09		C6H5BR1O1	P-BROMOPHENOL
1376	OLEYL ALCOHOL	124		2.23	2.77	C6H5BR1O1	P-BROMOPHENOL
1377	OCTANOL	10		2.84	2.84 =	C6H5CL1	CHLOROBENZENE
1378	OCTANOL	217	07	1.91	1.91 =	C6H5CL1N2O4S1	3-NITRO-4-CHLOROBENZENESULFONAMIOE
1379	CHCL3	217	07	0.03	1.21 A	C6H5CL1N2O4S1	3-NITRO-4-CHLOROBENZENESULFONAMIOE
1380	OCTANOL	10		2.50	2.50 =	C6H5CL1O1	M-CHLOROPHENOL
1381	OCTANOL	301		2.47	2.47 =	C6H5CL1O1	M-CHLOROPHENOL
1382	CYCLOHEXANE	124		-0.70		C6H5CL1O1	M-CHLOROPHENOL
1383	METH. OECANOATE	124		1.96	2.43	C6H5CL1O1	M-CHLOROPHENOL
1384	OLEYL ALCOHOL	124		1.76	2.31	C6H5CL1O1	M-CHLOROPHENOL
1385	OCTANOL	10		2.15	2.15 =	C6H5CL1O1	O-CHLOROPHENOL
1386	OCTANOL	301		2.19	2.19 =	C6H5CL1O1	O-CHLOROPHENOL
1387	CYCLOHEXANE	124		0.08		C6H5CL1O1	O-CHLOROPHENOL
1388	METH. OECANOATE	124		1.34	1.79	C6H5CL1O1	O-CHLOROPHENOL
1389	OLEYL ALCOHOL	124		1.23	1.78	C6H5CL1O1	O-CHLOROPHENOL
1390	OCTANOL	10		2.39	2.39 =	C6H5CL1O1	P-CHLOROPHENOL
1391	OCTANOL	301		2.44	2.44 =	C6H5CL1O1	P-CHLOROPHENOL
1392	CYCLOHEXANE	124		-0.70		C6H5CL1O1	P-CHLOROPHENOL
1393	CYCLOHEXANE	56		-0.26		C6H5CL1O1	P-CHLOROPHENOL
1394	METH. OECANOATE	124		2.18	2.65	C6H5CL1O1	P-CHLOROPHENOL
1395	OLEYL ALCOHOL	124		2.02	2.57	C6H5CL1O1	P-CHLOROPHENOL
1396	OCTANOL	268		2.78	2.78 =	C6H5CL2N1	2,3-OICHLOROANILINE
1397	OCTANOL	268		2.69	2.69 =	C6H5CL2N1	3,4-OICHLOROANILINE
1398	OCTANOL	217	07	1.44	1.44 =	C6H5CL2N1O2S1	3,4-OICHLOROBENZENESULFONAMIOE
1399	CHCL3	217	07	0.52	1.64 A	C6H5CL2N1O2S1	3,4-OICHLOROBENZENESULFONAMIOE
1400	OCTANOL	10		2.27	2.27 =	C6H5F1	FLUOROBENZENE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1401	OCTANOL	10		1.93	1.93 =	C6H5F1O1	M-FLUOROPHENOL
1402	CYCLOHEXANE	124		-1.00		C6H5F1O1	M-FLUOROPHENOL
1403	CYCLOHEXANE	300		-0.70		C6H5F1O1	M-FLUOROPHENOL
1404	METH. DECANOATE	124		1.56	2.02	C6H5F1O1	M-FLUOROPHENOL
1405	OLEYL ALCOHOL	124		1.43	1.98	C6H5F1O1	M-FLUOROPHENOL
1406	OLEYL ALCOHOL	300		1.73	2.28	C6H5F1O1	M-FLUOROPHENOL
1407	OCTANOL	10		1.71	1.71 =	C6H5F1O1	O-FLUOROPHENOL
1408	CYCLOHEXANE	124		-0.70		C6H5F1O1	O-FLUOROPHENOL
1409	CYCLOHEXANE	300		-0.15		C6H5F1O1	O-FLUOROPHENOL
1410	METH. DECANOATE	124		1.00	1.41	C6H5F1O1	O-FLUOROPHENOL
1411	OLEYL ALCOHOL	124		0.90	1.46	C6H5F1O1	O-FLUOROPHENOL
1412	OLEYL ALCOHOL	300		1.39	1.95	C6H5F1O1	O-FLUOROPHENOL
1413	OCTANOL	10		1.77	1.77 =	C6H5F1O1	P-FLUOROPHENOL
1414	CYCLOHEXANE	300		-1.00		C6H5F1O1	P-FLUOROPHENOL
1415	OLEYL ALCOHOL	124		1.49	2.04	C6H5F1O1	P-FLUOROPHENOL
1416	OLEYL ALCOHOL	300		1.48	2.03	C6H5F1O1	P-FLUOROPHENOL
1417	OCTANOL	56		3.25	3.25 =	C6H5I1	IODOBENZENE
1418	OCTANOL	10		2.93	2.93 =	C6H5I1O1	M-IODOPHENOL
1419	CYCLOHEXANE	124		-0.10		C6H5I1O1	M-IODOPHENOL
1420	METH. DECANOATE	124		2.41	2.89	C6H5I1O1	M-IODOPHENOL
1421	OLEYL ALCOHOL	124		2.23	2.77	C6H5I1O1	M-IODOPHENOL
1422	OCTANOL	10		2.65	2.65 =	C6H5I1O1	O-IODOPHENOL
1423	OLEYL ALCOHOL	124		1.79	2.34	C6H5I1O1	O-IODOPHENOL
1424	OCTANOL	10		2.91	2.91 =	C6H5I1O1	P-IODOPHENOL
1425	CYCLOHEXANE	124		0.00		C6H5I1O1	P-IODOPHENOL
1426	CYCLOHEXANE	56		0.21		C6H5I1O1	P-IODOPHENOL
1427	OLEYL ALCOHOL	124		2.59	3.13	C6H5I1O1	P-IODOPHENOL
1428	OCTANOL	56	26	-1.61	-1.61 =	C6H5I1O1	IODOXYBENZENE
1429	DIETHYL ETHER	306		-1.82	-1.46 A	C6H5I1O3S1	P-IODOBENZENESULFONIC ACID
1430	ETHYL ACETATE	306		-0.96	-1.08	C6H5I1O3S1	P-IODOBENZENESULFONIC ACID
1431	CLCH2CH2CL	306		-2.52		C6H5I1O3S1	P-IODOBENZENESULFONIC ACID
1432	OCTANOL	56		2.01	2.01 =	C6H5N1O1	NITROSOBENZENE
1433	OCTANOL	65		1.99	1.99 =	C6H5N1O1	NITROSOBENZENE
1434	DIETHYL ETHER	112	12	-2.05	-0.97 B	C6H5N1O2	2-CARBOXYPYRIDINE/PICOLINIC ACID/
1435	CHCL3	112	12	-1.64	-0.27 A	C6H5N1O2	2-CARBOXYPYRIDINE/PICOLINIC ACID/
1436	DIETHYL ETHER	112	50	-0.99	0.03 B	C6H5N1O2	3-CARBOXYPYRIDINE/NICOTINIC ACID/
1437	CHCL3	112	12	-2.05	-0.65 A	C6H5N1O2	3-CARBOXYPYRIDINE/NICOTINIC ACID/
1438	OCTANOL	10		1.85	1.85 =	C6H5N1O2	NITROBENZENE
1439	OCTANOL	301		1.88	1.88 =	C6H5N1O2	NITROBENZENE
1440	CYCLOHEXANE	141		1.46		C6H5N1O2S1	2-(B-NITROVINYL) THIOPHENE
1441	OCTANOL	10		2.00	2.00 =	C6H5N1O3	M-NITROPHENOL
1442	OCTANOL	301		2.00	2.00 =	C6H5N1O3	M-NITROPHENOL
1443	DIETHYL ETHER	3		2.20	2.05 A	C6H5N1O3	M-NITROPHENOL
1444	DIETHYL ETHER	112		2.18	2.02 A	C6H5N1O3	M-NITROPHENOL
1445	CYCLOHEXANE	248		-1.52		C6H5N1O3	M-NITROPHENOL
1446	CHCL3	307		0.41	1.59 A	C6H5N1O3	M-NITROPHENOL
1447	BENZENE	248		0.38	1.77 A	C6H5N1O3	M-NITROPHENOL
1448	1-BUTANOL	4		1.79	2.01	C6H5N1O3	M-NITROPHENOL
1449	CLCH2CH2CL	248		0.93		C6H5N1O3	M-NITROPHENOL
1450	OCTANOL	10		1.79	1.79 =	C6H5N1O3	O-NITROPHENOL
1451	OCTANOL	301		1.73	1.73 =	C6H5N1O3	O-NITROPHENOL
1452	DIETHYL ETHER	3		2.18	2.03 A	C6H5N1O3	O-NITROPHENOL
1453	CYCLOHEXANE	308		1.49		C6H5N1O3	O-NITROPHENOL
1454	CHCL3	307		2.54	1.97 B	C6H5N1O3	O-NITROPHENOL
1455	BENZENE	308		2.33	2.16 B	C6H5N1O3	O-NITROPHENOL
1456	I-BUTANOL	4		1.60	1.75	C6H5N1O3	O-NITROPHENOL
1457	XYLENE	308		2.30		C6H5N1O3	O-NITROPHENOL
1458	TOLUENE	308		2.28	3.58 A	C6H5N1O3	O-NITROPHENOL
1459	CCL4	308		2.07		C6H5N1O3	O-NITROPHENOL
1460	CS2	308		2.17		C6H5N1O3	O-NITROPHENOL
1461	OCTANOL	10		1.91	1.91 =	C6H5N1O3	P-NITROPHENOL
1462	OCTANOL	301		1.91	1.91 =	C6H5N1O3	P-NITROPHENOL
1463	DIETHYL ETHER	3		2.04	1.90 A	C6H5N1O3	P-NITROPHENOL
1464	DIETHYL ETHER	112		2.01	1.89 A	C6H5N1O3	P-NITROPHENOL
1465	CYCLOHEXANE	308		-1.93		C6H5N1O3	P-NITROPHENOL
1466	CYCLOHEXANE	248		-1.79		C6H5N1O3	P-NITROPHENOL
1467	CHCL3	307		0.08	1.29 A	C6H5N1O3	P-NITROPHENOL
1468	CHCL3	308		0.27	1.46 A	C6H5N1O3	P-NITROPHENOL
1469	BENZENE	308		0.15	1.56 A	C6H5N1O3	P-NITROPHENOL
1470	BENZENE	248		0.07	1.48 A	C6H5N1O3	P-NITROPHENOL
1471	I-BUTANOL	4		1.76	1.97	C6H5N1O3	P-NITROPHENOL
1472	CCL4	308		-0.99		C6H5N1O3	P-NITROPHENOL
1473	CCL4	234		-1.06		C6H5N1O3	P-NITROPHENOL
1474	CLCH2CH2CL	248		0.79		C6H5N1O3	P-NITROPHENOL
1475	HEXANE	308		-2.22		C6H5N1O3	P-NITROPHENOL
1476	CS2	308		-1.04		C6H5N1O3	P-NITROPHENOL
1477	CYCLOHEXANE	141		1.01		C6H5N1O3	2-(B-NITROVINYL) FURAN
1478	DIETHYL ETHER	112	12	-1.08	-0.82 A	C6H5N1O3	PICOLINIC ACID,N-OXIDE
1479	CHCL3	112		0.03	1.25 A	C6H5N1O3	PICOLINIC ACID,N-OXIDE
1480	OCTANOL	186		1.34	1.34 =	C6H5N3	BENZOTRIAZOLE
1481	DIETHYL ETHER	112		0.58	1.38 B	C6H5N3	BENZOTRIAZOLE
1482	CHCL3	112		-0.05	0.53 N	C6H5N3	BENZOTRIAZOLE
1483	OCTANOL	10		2.13	2.13 =	C6H6	BENZENE
1484	OCTANOL	309		1.56	1.56 =	C6H6	BENZENE
1485	OCTANOL	301		2.15	2.15 =	C6H6	BENZENE
1486	OILS	173		2.22	2.28 B	C6H6	BENZENE
1487	N-HEPTANE	310		2.26		C6H6	BENZENE
1488	BENZENE	311	6	0.10		C6H6B1BR1O2	PHENYLBORONIC ACID,4-BROMO
1489	BENZENE	311	6	-0.09		C6H6B1CL1O2	PHENYLBORONIC ACID,4-CHLORO
1490	BENZENE	311	6	-0.51		C6H6B1F1O2	PHENYLBORONIC ACID,4-FLUORO
1491	BENZENE	311	6	-1.09		C6H6B1N1O4	PHENYLBORONIC ACID,3-NITRO
1492	BENZENE	311	6	-0.82		C6H6B1N1O4	PHENYLBORONIC ACID,2-NITRO
1493	OCTANOL	312		2.10	2.10 =	C6H6BR1N1	M-BROMOANILINE
1494	BENZENE	313		2.20	2.07 B	C6H6BR1N1	M-BROMOANILINE
1495	OCTANOL	312		2.29	2.29 =	C6H6BR1N1	O-BROMOANILINE
1496	OCTANOL	312		2.26	2.26 =	C6H6BR1N1	P-BROMOANILINE
1497	BENZENE	313		2.06	1.98 B	C6H6BR1N1	P-BROMOANILINE
1498	BENZENE	72		2.12	2.09 B	C6H6BR1N1	P-BROMOANILINE
1499	OCTANOL	217	07	1.36	1.36 =	C6H6BR1N1O2S1	P-BROMOBENZENESULFONAMIDE
1500	CHCL3	217	07	0.39	0.92 N	C6H6BR1N1O2S1	P-BROMOBENZENESULFONAMIDE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1501	OCTANOL	10		1.88	1.88 =	C6H6CL1N1	M-CHLOROANILINE
1502	OCTANOL	301		1.90	1.90 =	C6H6CL1N1	M-CHLOROANILINE
1503	CYCLOHEXANE	314		0.89		C6H6CL1N1	M-CHLOROANILINE
1504	BENZENE	313		1.93	1.88 B	C6H6CL1N1	M-CHLOROANILINE
1505	BENZENE	315		1.94	1.91 B	C6H6CL1N1	M-CHLOROANILINE
1506	CCL4	314		1.37		C6H6CL1N1	M-CHLOROANILINE
1507	N-HEPTANE	314		0.71		C6H6CL1N1	M-CHLOROANILINE
1508	HEXADECANE	314		0.64		C6H6CL1N1	M-CHLOROANILINE
1509	OCTANOL	268		1.90	1.90 =	C6H6CL1N1	O-CHLOROANILINE
1510	OCTANOL	301		1.92	1.92 =	C6H6CL1N1	O-CHLOROANILINE
1511	CYCLOHEXANE	314		1.25		C6H6CL1N1	O-CHLOROANILINE
1512	BENZENE	314		2.13	2.02 B	C6H6CL1N1	O-CHLOROANILINE
1513	BENZENE	315		2.08	1.99 B	C6H6CL1N1	O-CHLOROANILINE
1514	CCL4	314		1.73		C6H6CL1N1	O-CHLOROANILINE
1515	N-HEPTANE	314		1.12		C6H6CL1N1	O-CHLOROANILINE
1516	HEXANE	314		1.11		C6H6CL1N1	O-CHLOROANILINE
1517	OCTANE	314		1.03		C6H6CL1N1	O-CHLOROANILINE
1518	HEXADECANE	314		1.07		C6H6CL1N1	O-CHLOROANILINE
1519	DECANE	314		1.12		C6H6CL1N1	O-CHLOROANILINE
1520	OCTANOL	301		1.83	1.83 =	C6H6CL1N1	P-CHLOROANILINE
1521	CYCLOHEXANE	314		0.69		C6H6CL1N1	P-CHLOROANILINE
1522	BENZENE	314		1.82	1.81 B	C6H6CL1N1	P-CHLOROANILINE
1523	BENZENE	313		1.81	1.80 B	C6H6CL1N1	P-CHLOROANILINE
1524	BENZENE	72		1.91	1.87 B	C6H6CL1N1	P-CHLOROANILINE
1525	BENZENE	315		1.80	1.80 B	C6H6CL1N1	P-CHLOROANILINE
1526	CCL4	314		1.31		C6H6CL1N1	P-CHLOROANILINE
1527	DI-PENTYL ETHER	315		0.64		C6H6CL1N1	P-CHLOROANILINE
1528	N-HEPTANE	75		0.63		C6H6CL1N1	P-CHLOROANILINE
1529	N-HEPTANE	314		0.57		C6H6CL1N1	P-CHLOROANILINE
1530	N-HEPTANE	315		0.64		C6H6CL1N1	P-CHLOROANILINE
1531	PARAFFINS	316		0.50		C6H6CL1N1	P-CHLOROANILINE
1532	HEXADECANE	314		0.56		C6H6CL1N1	P-CHLOROANILINE
1533	OCTANOL	217	07	1.29	1.29 =	C6H6CL1N1O2S1	M-CHLOROBENZENESULFONAMIDE
1534	CHCL3	217	07	0.26	0.89 N	C6H6CL1N1O2S1	M-CHLOROBENZENESULFONAMIDE
1535	OCTANOL	217	07	0.74	0.74 =	C6H6CL1N1O2S1	O-CHLOROBENZENESULFONAMIDE
1536	CHCL3	217	07	0.46	0.96 N	C6H6CL1N1O2S1	O-CHLOROBENZENESULFONAMIDE
1537	OCTANOL	217	07	0.84	0.84 =	C6H6CL1N1O2S1	P-CHLOROBENZENESULFONAMIDE
1538	CHCL3	217	07	0.14	0.69 N	C6H6CL1N1O2S1	P-CHLOROBENZENESULFONAMIDE
1539	HEXANE	317		3.24		C6H6CL6	1,2,3,4,5,6-HEXACHLOROCYCLOHEXANE /LINDANE/
1540	OCTANOL	312		1.30	1.30 =	C6H6F1N1	M-FLUOROANILINE
1541	OCTANOL	10		1.30	1.30 =	C6H6F1N1	M-FLUOROANILINE
1542	OCTANOL	312		1.26	1.26 =	C6H6F1N1	O-FLUOROANILINE
1543	OCTANOL	10		1.15	1.15 =	C6H6F1N1	P-FLUOROANILINE
1544	OCTANOL	312		2.98	2.98 =	C6H6I1N1	M-IODOANILINE
1545	OCTANOL	312	12	3.34	3.34 =	C6H6I1N1	O-IODOANILINE
1546	OCTANOL	312	12	3.34	3.34 =	C6H6I1N1	P-IODOANILINE
1547	DIETHYL ETHER	112		-1.72	-0.61 B	C6H6N2O1	NICOTINAMIDE/3-CARBAMYLPYRIDINE/
1548	CHCL3	112		-1.37	-1.40 B	C6H6N2O1	NICOTINAMIDE/3-CARBAMYLPYRIDINE/
1549	CHCL3	318		-1.22	-1.27 B	C6H6N2O1	I-NICOTINAMIDE
1550	OCTANOL	10		1.37	1.37 =	C6H6N2O2	M-NITROANILINE
1551	OCTANOL	301		1.37	1.37 =	C6H6N2O2	M-NITROANILINE
1552	DIETHYL ETHER	112		1.71	1.61 A	C6H6N2O2	M-NITROANILINE
1553	CYCLOHEXANE	319		-0.42		C6H6N2O2	M-NITROANILINE
1554	CYCLOHEXANE	314		-0.42		C6H6N2O2	M-NITROANILINE
1555	CHCL3	112		1.61	1.13 B	C6H6N2O2	M-NITROANILINE
1556	CHCL3	254		1.59	1.12 B	C6H6N2O2	M-NITROANILINE
1557	BENZENE	319		1.31	1.46 B	C6H6N2O2	M-NITROANILINE
1558	BENZENE	314		1.30	1.45 B	C6H6N2O2	M-NITROANILINE
1559	BENZENE	72		1.36	1.49 B	C6H6N2O2	M-NITROANILINE
1560	TOLUENE	319		1.19	1.49 B	C6H6N2O2	M-NITROANILINE
1561	CCL4	319		0.45	1.39 N	C6H6N2O2	M-NITROANILINE
1562	CCL4	314		0.43		C6H6N2O2	M-NITROANILINE
1563	N-HEPTANE	319		-0.57		C6H6N2O2	M-NITROANILINE
1564	N-HEPTANE	254		-0.62		C6H6N2O2	M-NITROANILINE
1565	N-HEPTANE	314		-0.56		C6H6N2O2	M-NITROANILINE
1566	OCTANE	314		-0.61		C6H6N2O2	M-NITROANILINE
1567	CS2	319		0.52		C6H6N2O2	M-NITROANILINE
1568	OCTANOL	312		1.44	1.44 =	C6H6N2O2	O-NITROANILINE
1569	OCTANOL	186		1.83	1.83 =	C6H6N2O2	O-NITROANILINE
1570	OCTANOL	301		1.79	1.79 =	C6H6N2O2	O-NITROANILINE
1571	DIETHYL ETHER	112	50	1.95	1.83 A	C6H6N2O2	O-NITROANILINE
1572	CYCLOHEXANE	319		0.36		C6H6N2O2	O-NITROANILINE
1573	CYCLOHEXANE	314		-0.70		C6H6N2O2	O-NITROANILINE
1574	CHCL3	112		2.13	1.60 B	C6H6N2O2	O-NITROANILINE
1575	BENZENE	319		1.78	1.79 B	C6H6N2O2	O-NITROANILINE
1576	BENZENE	72		1.81	1.81 B	C6H6N2O2	O-NITROANILINE
1577	TOLUENE	319		1.64	1.84 B	C6H6N2O2	O-NITROANILINE
1578	CCL4	319		1.08	2.25 N	C6H6N2O2	O-NITROANILINE
1579	CCL4	314		1.08		C6H6N2O2	O-NITROANILINE
1580	N-HEPTANE	319		0.25		C6H6N2O2	O-NITROANILINE
1581	N-HEPTANE	315		0.25		C6H6N2O2	O-NITROANILINE
1582	HEXANE	319		0.21		C6H6N2O2	O-NITROANILINE
1583	OLEYL ALCOHOL	82		1.15	1.71	C6H6N2O2	O-NITROANILINE
1584	CS2	319		1.14		C6H6N2O2	O-NITROANILINE
1585	OCTANOL	10		1.39	1.39 =	C6H6N2O2	P-NITROANILINE
1586	DIETHYL ETHER	112		1.48	1.41 A	C6H6N2O2	P-NITROANILINE
1587	CYCLOHEXANE	319		-1.00		C6H6N2O2	P-NITROANILINE
1588	CYCLOHEXANE	314		-1.00		C6H6N2O2	P-NITROANILINE
1589	CHCL3	112		1.23	0.78 B	C6H6N2O2	P-NITROANILINE
1590	CHCL3	254		1.30	0.89 B	C6H6N2O2	P-NITROANILINE
1591	BENZENE	319		0.92	1.19 B	C6H6N2O2	P-NITROANILINE
1592	BENZENE	314		0.93	1.19 B	C6H6N2O2	P-NITROANILINE
1593	BENZENE	72		0.95	1.21 B	C6H6N2O2	P-NITROANILINE
1594	TOLUENE	319		0.78	1.19 B	C6H6N2O2	P-NITROANILINE
1595	CCL4	319		-0.13	0.61 N	C6H6N2O2	P-NITROANILINE
1596	CCL4	314		-0.14		C6H6N2O2	P-NITROANILINE
1597	N-HEPTANE	319		-1.14		C6H6N2O2	P-NITROANILINE
1598	N-HEPTANE	254		-0.89		C6H6N2O2	P-NITROANILINE
1599	N-HEPTANE	314		-1.13		C6H6N2O2	P-NITROANILINE
1600	OCTANE	314		-1.25		C6H6N2O2	P-NITROANILINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1601	CS2	319		0.05		C6H6N2O2	P-NITROANILINE
1602	CS2	314		0.05		C6H6N2O2	P-NITROANILINE
1603	DIETHYL ETHER	320		1.80	1.70 A	C6H6N2O2	N-NITROSOPHENYLHYDROXYL AMINE
1604	CHCL3	321		2.15	2.64 N	C6H6N2O2	N-NITROSOPHENYLHYDROXYL AMINE
1605	ETHYL ACETATE	321		2.45	2.58	C6H6N2O2	N-NITROSOPHENYLHYDROXYL AMINE
1606	CCL4	320		3.36		C6H6N2O2	N-NITROSOPHENYLHYDROXYL AMINE
1607	N-BUTYL ACETATE	320		2.23	2.06	C6H6N2O2	N-NITROSOPHENYLHYDROXYLAMINE
1608	OCTANOL	217	07	0.55	0.55 =	C6H6N2O4S1	M-NITROBENZENESULFONAMIDE
1609	CHCL3	217	07	-0.36	0.85 A	C6H6N2O4S1	M-NITROBENZENESULFONAMIDE
1610	OCTANOL	217	07	0.34	0.34 =	C6H6N2O4S1	O-NITROBENZENESULFONAMIDE
1611	CHCL3	217	07	0.14	0.69 N	C6H6N2O4S1	O-NITROBENZENESULFONAMIDE
1612	OCTANOL	217	07	0.64	0.64 =	C6H6N2O4S1	P-NITROBENZENESULFONAMIDE
1613	CHCL3	217	07	-0.60	0.65 A	C6H6N2O4S1	P-NITROBENZENESULFONAMIDE
1614	DIETHYL ETHER	112	12	-0.05	0.07 A	C6H6N2S1	PYRIDINE,4-THIOCARBAMYL/1-NICOTINTHIOAMIDE/
1615	CHCL3	112		-0.41	-0.58 B	C6H6N2S1	PYRIDINE,4-THIOCARBAMYL/1-NICOTINTHIOAMIDE/
1616	CHCL3	322		-0.33	-0.39 B	C6H6N4S1	METHYLTHIOPURINE
1617	OCTANOL	10		1.46	1.46 =	C6H6O1	PHENOL
1618	OCTANOL	301		1.48	1.48 =	C6H6O1	PHENOL
1619	DIETHYL ETHER	3		1.64	1.55 A	C6H6O1	PHENOL
1620	DIETHYL ETHER	323		1.58	1.50 A	C6H6O1	PHENOL
1621	CYCLOHEXANE	124		-1.00		C6H6O1	PHENOL
1622	CYCLOHEXANE	132		-0.72		C6H6O1	PHENOL
1623	CYCLOHEXANE	324	45	-0.93		C6H6O1	PHENOL
1624	CYCLOHEXANE	325		-0.77		C6H6O1	PHENOL
1625	CYCLOHEXANE	56		-0.81		C6H6O1	PHENOL
1626	CYCLOHEXANE	300		-1.00		C6H6O1	PHENOL
1627	CHCL3	243		0.00	1.22 A	C6H6O1	PHENOL
1628	CHCL3	324	45	0.34	1.54 A	C6H6O1	PHENOL
1629	CHCL3	326		0.37	1.55 A	C6H6O1	PHENOL
1630	CHCL3	254		0.36	1.49 A	C6H6O1	PHENOL
1631	OILS	324		0.81	1.93 A	C6H6O1	PHENOL
1632	OILS	173		0.78	1.96 A	C6H6O1	PHENOL
1633	OILS	224		0.60	1.76 A	C6H6O1	PHENOL
1634	OILS	327		0.75	1.87 A	C6H6O1	PHENOL
1635	BENZENE	35		0.36	1.76 A	C6H6O1	PHENOL
1636	BENZENE	324	45	0.34	1.70 A	C6H6O1	PHENOL
1637	BENZENE	328		0.41	1.77 A	C6H6O1	PHENOL
1638	BENZENE	329		0.40	1.76 A	C6H6O1	PHENOL
1639	BENZENE	330		0.37	1.73 A	C6H6O1	PHENOL
1640	BENZENE	219		0.32	1.69 A	C6H6O1	PHENOL
1641	BENZENE	248		0.42	1.81 A	C6H6O1	PHENOL
1642	XYLENE	324	45	0.13	1.93 A	C6H6O1	PHENOL
1643	XYLENE	42		0.18	1.97 A	C6H6O1	PHENOL
1644	TOLUENE	324	45	0.22	1.77 A	C6H6O1	PHENOL
1645	TOLUENE	328		0.32	1.86 A	C6H6O1	PHENOL
1646	TOLUENE	42		0.23	1.75 A	C6H6O1	PHENOL
1647	NITROBENZENE	324	45	0.95	1.66	C6H6O1	PHENOL
1648	NITROBENZENE	328		0.87	1.60	C6H6O1	PHENOL
1649	PRIM. PENTANOLS	182		1.21	1.14	C6H6O1	PHENOL
1650	PRIM. PENTANOLS	324		1.50	1.55	C6H6O1	PHENOL
1651	N-BUTYL ACETATE	331		1.58	1.58	C6H6O1	PHENOL
1652	CCL4	324	45	-0.42	1.55 A	C6H6O1	PHENOL
1653	CCL4	328		-0.50	1.40 A	C6H6O1	PHENOL
1654	CCL4	329		-0.36	1.55 A	C6H6O1	PHENOL
1655	METH. DECANOATE	124		1.21	1.65	C6H6O1	PHENOL
1656	DI-I-PR. ETHER	331		1.12		C6H6O1	PHENOL
1657	N-HEPTANE	310		-0.92		C6H6O1	PHENOL
1658	N-HEPTANE	254		-0.82		C6H6O1	PHENOL
1659	HEXANE	324	45	-0.96		C6H6O1	PHENOL
1660	HEXANOL	331		1.46		C6H6O1	PHENOL
1661	OLEYL ALCOHOL	124		1.23	1.78	C6H6O1	PHENOL
1662	OLEYL ALCOHOL	300		1.19	1.75	C6H6O1	PHENOL
1663	CS2	248		-0.26		C6H6O1	PHENOL
1664	PARAFFINS	327		-0.85		C6H6O1	PHENOL
1665	BROMOFORM	7		0.18		C6H6O1	PHENOL
1666	OCTANOL	10		0.80	0.80 =	C6H6O2	M-DIHYDROXYBENZENE/RESORCINOL/
1667	OCTANOL	301		0.77	0.77 =	C6H6O2	M-DIHYDROXYBENZENE/RESORCINOL/
1668	DIETHYL ETHER	3		0.62	0.67 A	C6H6O2	M-DIHYDROXYBENZENE /RESORCINOL/
1669	DIETHYL ETHER	248		0.67	0.70 A	C6H6O2	M-DIHYDROXYBENZENE/RESORCINOL/
1670	BENZENE	248	12	-2.11		C6H6O2	M-DIHYDROXYBENZENE/RESORCINOL/
1671	N-BUTYL ACETATE	331		0.32	0.57	C6H6O2	M-DIHYDROXYBENZENE /RESORCINOL/
1672	CLCH2CH2CL	248		-1.50		C6H6O2	M-DIHYDROXYBENZENE/RESORCINOL/
1673	OCTANOL	56		0.88	0.88 =	C6H6O2	O-DIHYDROXYBENZENE/CATECHOL/
1674	OCTANOL	301		1.01	1.01 =	C6H6O2	O-DIHYDROXYBENZENE/CATECHOL/
1675	DIETHYL ETHER	3		1.04	1.03 A	C6H6O2	O-DIHYDROXYBENZENE/CATECHOL/
1676	DIETHYL ETHER	332		0.86	0.87 A	C6H6O2	O-DIHYDROXYBENZENE /CATECHOL/
1677	DIETHYL ETHER	323		0.89	0.90 A	C6H6O2	O-DIHYDROXYBENZENE/CATECHOL/
1678	BENZENE	248	12	-1.19	0.21 A	C6H6O2	O-DIHYDROXYBENZENE/CATECHOL/
1679	CLCH2CH2CL	248		-0.63		C6H6O2	O-DIHYDROXYBENZENE/CATECHOL/
1680	DI-BUTYL ETHER	332		0.11		C6H6O2	O-DIHYDROXYBENZENE /CATECHOL/
1681	DI-I-PR. ETHER	332		0.62	1.27	C6H6O2	O-DIHYDROXYBENZENE /CATECHOL/
1682	OCTANOL	302		0.59	0.59 =	C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1683	OCTANOL	301		0.50	0.50 =	C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1684	DIETHYL ETHER	3		0.46	0.51 A	C6H6O2	P-DIHYDROXYBENZENE /HYDROQUINONE/
1685	DIETHYL ETHER	333		0.36	0.44 A	C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1686	DIETHYL ETHER	334		0.37	0.45 A	C6H6O2	P-DIHYDROXYBENZENE /HYDROQUINONE/
1687	DIETHYL ETHER	248		0.38	0.44 A	C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1688	OILS	305		-0.83	-0.48 A	C6H6O2	P-DIHYDROXYBENZENE /HYDROQUINONE/
1689	BENZENE	248	12	-2.16		C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1690	CLCH2CH2CL	248		-1.61		C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1691	DI-I-PR. ETHER	335		-0.13	0.39	C6H6O2	P-DIHYDROXYBENZENE/HYDROQUINONE/
1692	CHCL3	336		-0.22	0.40 N	C6H6O3	2-FURALDEHYDE,HYDROXYMETHYL
1693	BENZENE	336	12	-0.24	1.04 A	C6H6O3	2-FURALDEHYDE,HYDROXYMETHYL
1694	ETHYL ACETATE	336		0.13	0.12	C6H6O3	2-FURALDEHYDE,5-HYDROXYMETHYL
1695	DIETHYL ETHER	3		0.23	0.32 A	C6H6O3	1,2,3-TRIHYDROXYBENZENE/PYROGALLOL/
1696	DIETHYL ETHER	248		0.09	0.19 A	C6H6O3	1,2,3-TRIHYDROXYBENZENE/PYROGALLOL/
1697	DIETHYL ETHER	3		-0.35	-0.19 A	C6H6O3	1,3,5-TRIHYDROXYBENZENE/PHLOROGLUCINOL/
1698	DIETHYL ETHER	248		-0.35	-0.19 A	C6H6O3	1,3,5-TRIHYDROXYBENZENE/PHLOROGLUCINOL/
1699	DIETHYL ETHER	3		-2.70	-2.25 A	C6H6O3S1	BENZENESULFONIC ACID
1700	DIETHYL ETHER	3		-0.30	-0.15 A	C6H6O6	ACONITIC ACID

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1701	DIETHYL ETHER	207		-0.62	-0.43 A	C6H6O6	ACONITIC ACID
1702	I-BUTANOL	4		0.49	0.18	C6H6O6	ACONITIC ACID
1703	ME-I-BUT.KETONE	195		-0.26	-0.24	C6H6O6	ACONITIC ACID
1704	OCTANOL	235		2.52	2.52 =	C6H6S1	THIOPHENOL
1705	OCTANOL	255		1.58	1.58 =	C6H7B1O2	PHENYLBORONIC ACID
1706	BENZENE	311	6	-0.80		C6H7B1O2	PHENYLBORONIC ACID
1707	BENZENE	311	6	-2.92		C6H7B1O3	PHENYLBORONIC ACID,4-HYDROXY
1708	BENZENE	311	6	-2.78		C6H7B1O3	PHENYLBORONIC ACID,3-HYDROXY
1709	BENZENE	311	6	-2.65		C6H7B2N1O6	PHENYL,1,4-DIBORONIC ACID,,2-NITRO
1710	OCTANOL	10		0.90	0.90 =	C6H7N1	ANILINE
1711	OCTANOL	301		0.98	0.98 =	C6H7N1	ANILINE
1712	DIETHYL ETHER	329		0.85	0.87 A	C6H7N1	ANILINE
1713	CYCLOHEXANE	337		0.02		C6H7N1	ANILINE
1714	CHCL3	254		1.42	0.98 B	C6H7N1	ANILINE
1715	CHCL3	338		1.23	0.82 B	C6H7N1	ANILINE
1716	BENZENE	338	12	-0.05		C6H7N1	ANILINE
1717	BENZENE	72		1.00	1.24 B	C6H7N1	ANILINE
1718	XYLENE	46		0.18	0.75 B	C6H7N1	ANILINE
1719	TOLUENE	339		0.89	1.30 B	C6H7N1	ANILINE
1720	CCL4	329		0.25	1.11 N	C6H7N1	ANILINE
1721	CLCH2CH2CL	248		1.45		C6H7N1	ANILINE
1722	N-HEPTANE	310		-0.03		C6H7N1	ANILINE
1723	N-HEPTANE	254		0.04		C6H7N1	ANILINE
1724	N-HEPTANE	338	44	-0.26		C6H7N1	ANILINE
1725	N-HEPTANE	340		0.04		C6H7N1	ANILINE
1726	PARAFFINS	316		-0.12		C6H7N1	ANILINE
1727	CHCL3	280		1.79	1.06 B	C6H7N1	2-METHYL PYRIDINE/2-PICOLINE/
1728	CHCL3	280		1.89		C6H7N1	3-METHYL PYRIDINE/3-PICOLINE/
1729	CHCL3	280		1.88		C6H7N1	4-METHYL PYRIDINE/4-PICOLINE/
1730	OCTANOL	276		1.20	1.20 =	C6H7N1	3-METHYLPYRIDINE /PKA = 5.68/
1731	OCTANOL	276		1.22	1.22 =	C6H7N1	4-METHYLPYRIDINE /PKA = 6.02/
1732	OCTANOL	10		0.17	0.17 =	C6H7N1O1	M-AMINOPHENOL
1733	OCTANOL	301		0.15	0.15 =	C6H7N1O1	M-AMINOPHENOL
1734	DIETHYL ETHER	248		0.11	0.22 A	C6H7N1O1	M-AMINOPHENOL
1735	CYCLOHEXANE	314		-3.24		C6H7N1O1	M-AMINOPHENOL
1736	BENZENE	314		-1.36	0.04 A	C6H7N1O1	M-AMINOPHENOL
1737	BENZENE	248		-1.32	0.08 A	C6H7N1O1	M-AMINOPHENOL
1738	CCL4	314		-2.39	-0.19 A	C6H7N1O1	M-AMINOPHENOL
1739	CLCH2CH2CL	248		-0.58		C6H7N1O1	M-AMINOPHENOL
1740	N-HEPTANE	314		-3.37		C6H7N1O1	M-AMINOPHENOL
1741	HEXADECANE	314		-3.37		C6H7N1O1	M-AMINOPHENOL
1742	OCTANOL	56		0.62	0.62 =	C6H7N1O1	O-AMINOPHENOL
1743	OCTANOL	301		0.52	0.52 =	C6H7N1O1	O-AMINOPHENOL
1744	CYCLOHEXANE	314		-2.37		C6H7N1O1	O-AMINOPHENOL
1745	BENZENE	314		-0.84	0.55 A	C6H7N1O1	O-AMINOPHENOL
1746	CCL4	314		-1.75	0.37 A	C6H7N1O1	O-AMINOPHENOL
1747	N-HEPTANE	314		-2.51		C6H7N1O1	O-AMINOPHENOL
1748	OCTANOL	301		0.04	0.04 =	C6H7N1O1	P-AMINOPHENOL
1749	CYCLOHEXANE	314		-3.44		C6H7N1O1	P-AMINOPHENOL
1750	BENZENE	314		-1.65	-0.24 A	C6H7N1O1	P-AMINOPHENOL
1751	CCL4	314		-2.64	-0.39 A	C6H7N1O1	P-AMINOPHENOL
1752	N-HEPTANE	314		-3.55		C6H7N1O1	P-AMINOPHENOL
1753	OCTANOL	217	07	0.31	0.31 =	C6H7N1O2S1	BENZENESULFONAMIDE
1754	OCTANOL	10		0.31	0.31 =	C6H7N1O2S1	BENZENESULFONAMIDE
1755	DIETHYL ETHER	113		0.30	0.38 A	C6H7N1O2S1	BENZENESULFONAMIDE
1756	CHCL3	113		-0.24	0.34 N	C6H7N1O2S1	BENZENESULFONAMIDE
1757	CHCL3	217	07	-0.24	0.35 N	C6H7N1O2S1	BENZENESULFONAMIDE
1758	DIETHYL ETHER	113	16	0.82	0.83 A	C6H7N1O3S1	N-HYDROXYBENZENESULFONAMIDE
1759	CHCL3	113	16	-0.82	-0.16 N	C6H7N1O3S1	N-HYDROXYBENZENESULFONAMIDE
1760	OCTANOL	276		-0.50	-0.50 =	C6H7N3O1	4-CARBAMYLAMINOPYRIDINE
1761	CHCL3	322		-1.05	-0.95 B	C6H7N5	6-METHYLAMINOPURINE
1762	CHCL3	322		-0.95	-0.89 B	C6H7N5S1	2-AMINO-6-METHYLTHIOPURINE
1763	OCTANOL	276		1.39	1.39 =	C6H7O1	2-METHOXYPYRIDINE /PKA = 3.28/
1764	BENZENE	311	6	-2.32		C6H8B1N1O2	PHENYLBORONIC ACID,3-AMINO
1765	BENZENE	311	6	-2.61		C6H8B2O4	PHENYL,1,4-DIBORONIC ACID
1766	OCTANOL	276		1.02	1.02 =	C6H8N1	2-AMINO-5-METHYLPYRIDINE /PKA = 7.22/
1767	OCTANOL	276		0.62	0.62 =	C6H8N2	4,6-DIMETHYLPYRIMIDINE
1768	CYCLOHEXANE	314		-2.44		C6H8N2	M-PHENYLENEDIAMINE
1769	BENZENE	71		-0.79	0.00 B	C6H8N2	M-PHENYLENEDIAMINE
1770	BENZENE	314		-0.77	0.02 B	C6H8N2	M-PHENYLENEDIAMINE
1771	BENZENE	72		-0.75	0.03 B	C6H8N2	M-PHENYLENEDIAMINE
1772	BENZENE	248		-0.75	0.03 B	C6H8N2	M-PHENYLENEDIAMINE
1773	CCL4	314		-2.49		C6H8N2	M-PHENYLENEDIAMINE
1774	N-HEPTANE	314		-2.60		C6H8N2	M-PHENYLENEDIAMINE
1775	OCTANOL	301		0.15	0.15 =	C6H8N2	O-PHENYLENEDIAMINE
1776	DIETHYL ETHER	248		-0.06	0.08 A	C6H8N2	O-PHENYLENEDIAMINE
1777	CYCLOHEXANE	314		-1.65		C6H8N2	O-PHENYLENEDIAMINE
1778	CYCLOHEXANE	248	43	-1.31		C6H8N2	O-PHENYLENEDIAMINE
1779	BENZENE	71		-0.28	0.35 B	C6H8N2	O-PHENYLENEDIAMINE
1780	BENZENE	314		-0.26	0.37 B	C6H8N2	O-PHENYLENEDIAMINE
1781	BENZENE	72		-0.26	0.37 B	C6H8N2	O-PHENYLENEDIAMINE
1782	BENZENE	248		-0.26	0.37 B	C6H8N2	O-PHENYLENEDIAMINE
1783	CCL4	314		-0.81		C6H8N2	O-PHENYLENEDIAMINE
1784	CLCH2CH2CL	248		0.44		C6H8N2	O-PHENYLENEDIAMINE
1785	N-HEPTANE	314		-1.79		C6H8N2	O-PHENYLENEDIAMINE
1786	CYCLOHEXANE	314		-2.81		C6H8N2	P-PHENYLENEDIAMINE
1787	BENZENE	71		-1.17	-0.26 B	C6H8N2	P-PHENYLENEDIAMINE
1788	BENZENE	314		-1.17	-0.26 B	C6H8N2	P-PHENYLENEDIAMINE
1789	CCL4	314		-1.78		C6H8N2	P-PHENYLENEDIAMINE
1790	N-HEPTANE	314		-3.00		C6H8N2	P-PHENYLENEDIAMINE
1791	OCTANOL	283		1.25	1.25 =	C6H8N2	PHENYLHYDRAZINE
1792	OCTANOL	341	60	-0.10	-0.10 =	C6H8N2	3-PYRIDYLMETHYLAMINE
1793	OCTANOL	217	32	-0.83	-0.83 =	C6H8N2O2S1	SULFANILAMIDE
1794	OCTANOL	186		-0.72	-0.72 =	C6H8N2O2S1	SULFANILAMIDE
1795	DIETHYL ETHER	342		-0.72	-0.52 A	C6H8N2O2S1	SULFANILAMIDE
1796	DIETHYL ETHER	113		-0.85	-0.63 A	C6H8N2O2S1	SULFANILAMIDE
1797	CHCL3	343	2	-1.40	-0.70 N	C6H8N2O2S1	SULFANILAMIDE
1798	CHCL3	113		-1.63	-0.92 N	C6H8N2O2S1	SULFANILAMIDE
1799	CHCL3	344	44	-1.85	-1.07 N	C6H8N2O2S1	SULFANILAMIDE
1800	CHCL3	254		-1.52	-0.79 N	C6H8N2O2S1	SULFANILAMIDE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1801	CHCL3	217	32	-1.69	-0.97 N	C6H8N2O2S1	SULFANILAMIDE
1802	BENZENE	343	2	-2.05	-0.64 A	C6H8N2O2S1	SULFANILAMIDE
1803	1-BUTANOL	130	12	-0.96	-1.85	C6H8N2O2S1	SULFANILAMIDE
1804	1-PENT. ACETATE	343	2	-0.44	-0.67	C6H8N2O2S1	SULFANILAMIDE
1805	CCL4	343	2	-2.52	-0.29 A	C6H8N2O2S1	SULFANILAMIDE
1806	OILS	345		-1.18	0.16 A	C6H8N2O3	BARBITURIC ACID,DIMETHYL
1807	OILS	240		1.61	1.94 B	C6H8N2O8	ISOSORBIDE DINITRATE
1808	OILS	240		2.69	2.94 B	C6H8N6O18	MANNITOL HEXANITRATE
1809	OCTANOL	346		0.58	0.58 =	C6H8O1	1-HEXYN-5-ONE
1810	OILS	347		0.49	1.70 A	C6H8O2	SORBIC ACID
1811	ME-I-BUT.KETONE	195		1.10	0.96	C6H8O2	SORBIC ACID
1812	S-PENTANOLS	195		-0.30	-0.65	C6H8O6	PROPANE TRICARBOXYLIC ACID
1813	DIETHYL ETHER	3		-1.22	-0.95 A	C6H8O6	PROPANE TRICARBOXYLIC ACID
1814	DIETHYL ETHER	207		-1.30	-1.03 A	C6H8O6	PROPANE TRICARBOXYLIC ACID
1815	ME-I-BUT.KETONE	195		-1.00	-0.93	C6H8O6	PROPANE TRICARBOXYLIC ACID
1816	OLEYL ALCOHOL	5		-1.52	-0.94	C6H8O6	PROPANE TRICARBOXYLIC ACID
1817	1-BUTANOL	4		0.01	-0.49	C6H8O6	PROPANETRICARBOXYLIC ACID
1818	OCTANOL	5		-1.72	-1.72 =	C6H8O7	CITRIC ACID
1819	DIETHYL ETHER	3		-2.06	-1.69 A	C6H8O7	CITRIC ACID
1820	DIETHYL ETHER	207		-2.18	-1.80 A	C6H8O7	CITRIC ACID
1821	DIETHYL ETHER	213		-2.19	-1.79 A	C6H8O7	CITRIC ACID
1822	1-BUTANOL	4		-0.53	-1.25	C6H8O7	CITRIC ACID
1823	1-BUTANOL	184		-0.62	-1.38	C6H8O7	CITRIC ACID
1824	PRIM. PENTANOLS	48		-0.76	-1.27	C6H8O7	CITRIC ACID
1825	CYCLOHEXANONE	194		-0.67	-1.47	C6H8O7	CITRIC ACID
1826	2-BUTANONE	194		-0.48	-1.63	C6H8O7	CITRIC ACID
1827	ME-I-BUT.KETONE	195		-1.62	-1.51	C6H8O7	CITRIC ACID
1828	S-PENTANOLS	195		-1.16	-1.63	C6H8O7	CITRIC ACID
1829	OCTANOL	348		-0.70	-0.70 =	C6H9N1O2	N-FORMYLCYCLOBUTANECARBOXAMIDE
1830	OILS	284		0.19	0.95 B	C6H9N3O1	1,3,5-TRIMETHYL-4-NITROSOPYRAZOLE
1831	SEC-BUTANOL	84	19	-1.68	-2.86	C6H9N3O2	HISTIDINE
1832	OCTANE	256		-1.26		C6H9N3O2	2-I-PROPYL-5-NITROIMIDAZOLE
1833	OCTANOL	56		2.45	2.45 =	C6H10	1,5-HEXADIENE
1834	CHCL3	265		-0.94	-0.28 N	C6H10N2O2	CYCLOHEXANEDIONE DIOXIME
1835	OCTANOL	206		3.75	3.75 =	C6H10N2O6S3	IMIDAZOLE,2,4,5-TRIMETHYLSULFONYL
1836	OCTANOL	134		1.22	1.22 =	C6H10N4O1S1	3-MERCAPTO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
1837	OCTANOL	134		0.46	0.46 =	C6H10N4O1S1	3-METHIO-4-AMINO-6-ETHYL-1,2,4-TRIAZINE-5-ONE
1838	OCTANOL	349		-0.24	-0.24 =	C6H10N6O1	IMIDAZOLE-4-CARBOXAMIDE,5-(3,3-DIME-1-TRIAZENO)(45388)
1839	OCTANOL	65		0.81	0.81 =	C6H10O1	CYCLOHEXANONE
1840	OILS	258		0.30	0.69 B	C6H10O1	DIALLYL ETHER
1841	OCTANOL	255		1.02	1.02 =	C6H10O1	1-HEXEN-5-ONE
1842	50%ETHER+50%DMF	125		0.40	1.80	C6H10O1	3-METHYL-1-PENTYN-3-OL/MEPARFYNOL/
1843	CCL4	350		1.42	1.24 B	C6H10O1	1-PROPYLIDENE-ACETONE/MESITYL OXIDE/
1844	CHCL3	285		1.75	2.81 A	C6H10O2	2,4-HEXANEDIONE/PROPIONYLACETONE/
1845	DIETHYL ETHER	2		-0.35	-0.19 A	C6H10O2	2,5-HEXANEDIONE/ACETONYLACETONE/
1846	OILS	2		-1.09	0.17 A	C6H10O2	2,5-HEXANEDIONE/ACETONYLACETONE/
1847	OILS	173		0.04	1.23 A	C6H10O3	ETHYLACETOACETATE
1848	OCTANOL	255		-0.13	-0.13 =	C6H10O3	4-KETOVALERIC ACID,METHYL ESTER
1849	OCTANOL	5		0.08	0.08 =	C6H10O4	ADIPIC ACID
1850	DIETHYL ETHER	192		-0.29	-0.14 A	C6H10O4	ADIPIC ACID
1851	DIETHYL ETHER	351		-0.29	-0.14 A	C6H10O4	ADIPIC ACID
1852	DIETHYL ETHER	194		-0.24	-0.09 A	C6H10O4	ADIPIC ACID
1853	N-BUTANOL	194		0.44	0.09	C6H10O4	ADIPIC ACID
1854	1-BUTANOL	4		0.55	0.27	C6H10O4	ADIPIC ACID
1855	ETHYL ACETATE	194		0.08	0.05	C6H10O4	ADIPIC ACID
1856	CYCLOHEXANONE	194		0.49		C6H10O4	ADIPIC ACID
1857	2-BUTANONE	194		0.30	-0.06	C6H10O4	ADIPIC ACID
1858	ME-I-BUT.KETONE	194		-0.08	-0.82	C6H10O4	ADIPIC ACID
1859	ME-I-BUT.KETONE	195		-0.11	-0.16	C6H10O4	ADIPIC ACID
1860	S-PENTANOLS	195		0.48	0.24	C6H10O4	ADIPIC ACID
1861	DIETHYL ETHER	3		0.30	0.38 A	C6H10O4	ETHYLENE GLYCOL DIACETATE
1862	1-BUTANOL	4		0.43	0.10	C6H10O4	ETHYLENE GLYCOL DIACETATE
1863	OILS	352		0.30	1.46 A	C6H11BR1N2O2	A-BROMO-A-METHYLBUTYRYLUREA
1864	OILS	264		0.28	1.44 A	C6H11BR1N2O2	A-BROMO-A-METHYLBUTYRYLUREA
1865	OILS	264		0.12	1.30 A	C6H11BR1N2O2	A-BROMO-I-VALERYLUREA
1866	OILS	296		0.15	1.37 A	C6H11BR1N2O2	A-BROMO-I-VALERYLUREA/BROMISOVALUM/
1867	OILS	352		-0.36	0.87 A	C6H11BR1N2O2	A-BROMOVALERYLUREA
1868	OILS	264		-0.19	1.01 A	C6H11BR1N2O2	A-BROMOVALERYLUREA
1869	OILS	352		-0.45	0.78 A	C6H11BR1N2O2	B-BROMOVALERYLUREA
1870	OILS	352		-0.54	0.70 A	C6H11BR1N2O2	G-BROMOVALERYLUREA
1871	OILS	352		-0.07	1.13 A	C6H11BR1N2O2	A-ETHYL-B-BROMOPROPIONYLUREA
1872	OILS	352		0.23	1.39 A	C6H11BR1N2O2	A-METHYL-B-BROMOBUTRYLUREA
1873	OILS	352		-0.04	1.16 A	C6H11BR1N2O2	A-METHYL-G-BROMOBUTYRYLUREA
1874	OILS	264		-0.11	1.09 A	C6H11CL1N2O2	A-CHLORO-I-VALERYLUREA
1875	OILS	264		0.02	1.21 A	C6H11I1N2O2	A-IODO-I-VALERYLUREA
1876	I-OCTANOL	353		-2.60		C6H11K1O2	POTASSIUM HEXANOATE
1877	OCTANOL	260		-0.19	-0.19 =	C6H11N1O1	2-AZACYCLOHEPTANONE
1878	OCTANOL	80		1.09	1.09 =	C6H11N1O2	O-(1-ETHYL-ALLYL)CARBAMATE
1879	CYCLOHEXANE	354		-0.10		C6H11N1O2	NITROCYCLOHEXANE
1880	CHCL3	67		-1.60		C6H11N1O3	A-AMINOBUTYRIC ACID,N-ACETYL(DL)
1881	ETHYL ACETATE	67		-0.84	-0.96	C6H11N1O3	A-AMINOBUTYRIC ACID,N-ACETYL(DL)
1882	OCTANOL	260		0.75	0.75 =	C6H11N1S1	2-AZACYCLOHEPTANTHIONE
1883	OCTANOL	56		-2.17	-2.17 =	C6H11NA1O2	HEXANOIC ACID, SODIUM SALT
1884	I-OCTANOL	353		-2.59		C6H11NA1O2	SODIUM HEXANOATE
1885	OILS	296		0.42	1.57 A	C6H12BR1N1O1	2-BROMO-2-ETHYLBUTYRAMIDE
1886	OCTANOL	227		0.29	0.29 =	C6H12BR2O4	1,6-DIBROMO-1,6-DIDEOXYGALACTITOL (104800)
1887	OCTANOL	227		0.24	0.24 =	C6H12BR2O4	1,6-DIBROMO-1,6-DIDEOXYMANNITOL(94100)
1888	OCTANOL	216		0.04	0.04 =	C6H12N2O1	1-(2-HYDROXYETHYL)-2-METHYLIMIDAZOLINE
1889	OILS	264		-0.31	0.91 A	C6H12N2O2	VALERYLUREA
1890	OILS	264		-0.16	1.04 A	C6H12N2O2	I-VALERYLUREA
1891	OILS	2		-3.68	-2.13 A	C6H12N4	HEXAMETHYLENE TETRAMINE
1892	DIETHYL ETHER	2		-3.58	-2.34 B	C6H12N4	HEXAMETHYLENETETRAMINE
1893	I-BUTANOL	4		-1.17	-2.15	C6H12N4	HEXAMETHYLENETETRAMINE
1894	OCTANOL	186		1.23	1.23 =	C6H12O1	CYCLOHEXANOL
1895	OCTANOL	255		1.38	1.38 =	C6H12O1	2-HEXANONE
1896	OCTANOL	218		1.88	1.88 =	C6H12O2	HEXANOIC ACID
1897	OCTANOL	218		1.92	1.92 =	C6H12O2	HEXANOIC ACID
1898	DIETHYL ETHER	190		1.88	1.76 A	C6H12O2	HEXANOIC ACID
1899	DIETHYL ETHER	3		1.97	1.84 A	C6H12O2	HEXANOIC ACID
1900	DIETHYL ETHER	49		1.95	1.84 A	C6H12O2	HEXANOIC ACID

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
1901	CHCL3	29		1.05	2.19 A	C6H12O2	HEXANOIC ACIO
1902	CHCL3	46		0.85	1.99 A	C6H12O2	HEXANOIC ACIO
1903	OILS	209		0.83	2.01 A	C6H12O2	HEXANOIC ACIO
1904	BENZENE	44		0.67	2.06 A	C6H12O2	HEXANOIC ACIO
1905	BENZENE	29		0.63	2.02 A	C6H12O2	HEXANOIC ACIO
1906	N-BUTANOL	190		1.86	2.12	C6H12O2	HEXANOIC ACIO
1907	1-BUTANOL	4		1.87	2.12	C6H12O2	HEXANOIC ACIO
1908	1-BUTANOL	184		1.89	2.15	C6H12O2	HEXANOIC ACIO
1909	SEC-BUTANOL	190		1.39	1.46	C6H12O2	HEXANOIC ACIO
1910	XYLENE	46		0.34	2.06 A	C6H12O2	HEXANOIC ACIO
1911	TOLUENE	29		0.56	2.07 A	C6H12O2	HEXANOIC ACIO
1912	TOLUENE	7	26	1.03	2.48 A	C6H12O2	HEXANOIC ACIO
1913	PRIM. PENTANOLS	190		2.04	2.24	C6H12O2	HEXANOIC ACIO
1914	2-BUTANONE	190		1.36	2.13	C6H12O2	HEXANOIC ACIO
1915	OCTANE	60	47	-0.52		C6H12O2	HEXANOIC ACIO
1916	OLEYL ALCOHOL	5		1.65	2.20	C6H12O2	HEXANOIC ACIO
1917	S-PENTANOLS	190		1.94	1.93	C6H12O2	HEXANOIC ACIO
1918	OOOECANE	60	47	-0.72		C6H12O2	HEXANOIC ACIO
1919	HEXAOECANE	60	47	-0.85		C6H12O2	HEXANOIC ACIO
1920	IOOOMETHANE	7	26	0.81		C6H12O2	HEXANOIC ACIO
1921	OECALIN	7	26	-0.23		C6H12O2	HEXANOIC ACIO
1922	CHCL3	29		0.90	2.03 A	C6H12O2	I-HEXANOIC ACIO
1923	OILS	220		0.90	2.02 A	C6H12O2	I-HEXANOIC ACIO
1924	BENZENE	29		0.57	1.96 A	C6H12O2	I-HEXANOIC ACIO
1925	XYLENE	46		0.18	1.89 A	C6H12O2	I-HEXANOIC ACIO
1926	OIETHYL ETHER	2		0.95	0.95 A	C6H12O3	PARALOEHYOE
1927	OILS	2		0.28	0.70 B	C6H12O3	PARALOEHYOE
1928	OILS	173		0.28	0.59 B	C6H12O3	PARALOEHYOE
1929	OILS	296		0.45	0.70 B	C6H12O3	PARALOEHYOE
1930	1-BUTANOL	4		-1.24	-2.24	C6H12O5	RHAMNOSE
1931	1-BUTANOL	4		-1.77	-3.00	C6H12O6	FRUCTOSE
1932	1-BUTANOL	4		-1.96	-3.29	C6H12O6	GLUCOSE
1933	1-BUTANOL	4	11	-1.47	-2.57	C6H12O7	GLUCONIC ACIO
1934	OCTANOL	216	46	-1.93	-1.93 =	C6H13CL1N2O1	1-(2-HYOROXYETHYL)-2-METHYLIMIOAZOLINE HCL
1935	XYLENE	46		0.33	0.94 B	C6H13N1	N-METHYLPIPERIOINE
1936	CCL4	234	12	-0.45		C6H13N1O1	OIETHYLACETAMIOE
1937	N-BUTANOL	225		-0.51	-1.22	C6H13N1O2	A-AMINOCAPROIC ACIO
1938	OCTANOL	56		-1.71	-1.71 =	C6H13N1O2	LEUCINE
1939	OIETHYL ETHER	3		-4.92	-3.46 B	C6H13N1O2	LEUCINE
1940	N-BUTANOL	225		-0.74	-1.55	C6H13N1O2	LEUCINE
1941	I-BUTANOL	4		-1.21	-2.21	C6H13N1O2	LEUCINE
1942	OCTANOL	181	10	-0.15	-0.15 =	C6H13O9P1	FRUCTOSE-6-PHOSPHATE
1943	N-BUTANOL	181	10	-1.52		C6H13O9P1	FRUCTOSE-6-PHOSPHATE
1944	PRIM. PENTANOLS	181	10	-0.70		C6H13O9P1	FRUCTOSE-6-PHOSPHATE
1945	HEXANOL	181	18	-0.82		C6H13O9P1	FRUCTOSE-6-PHOSPHATE
1946	OCTANOL	181	10	-1.00	-1.00 =	C6H13O9P1	GLUCOSE-1-PHOSPHATE
1947	PRIM. PENTANOLS	181	10	-1.00		C6H13O9P1	GLUCOSE-1-PHOSPHATE
1948	OCTANOL	181	10	-0.10	-0.10 =	C6H13O9P1	GLUCOSE-6-PHOSPHATE
1949	N-BUTANOL	181	10	-1.05		C6H13O9P1	GLUCOSE-6-PHOSPHATE
1950	PRIM. PENTANOLS	181	10	-1.00		C6H13O9P1	GLUCOSE-6-PHOSPHATE
1951	HEXANOL	181	18	-0.40		C6H13O9P1	GLUCOSE-6-PHOSPHATE
1952	OCTANOL	181	10	-0.10	-0.10 =	C6H13O9P1	SORBOSE-1-PHOSPHATE
1953	N-BUTANOL	181	10	-0.30		C6H13O9P1	SORBOSE-1-PHOSPHATE
1954	PRIM. PENTANOLS	181	10	-1.40		C6H13O9P1	SORBOSE-1-PHOSPHATE
1955	HEXANOL	181	18	-1.00		C6H13O9P1	SORBOSE-1-PHOSPHATE
1956	OCTANOL	181	10	0.38	0.38 =	C6H13O9P1	SORBOSE-6-PHOSPHATE
1957	N-BUTANOL	181	10	-1.00		C6H13O9P1	SORBOSE-6-PHOSPHATE
1958	PRIM. PENTANOLS	181	10	-0.05		C6H13O9P1	SORBOSE-6-PHOSPHATE
1959	HEXANOL	181	18	0.26		C6H13O9P1	SORBOSE-6-PHOSPHATE
1960	N-BUTANOL	295	52	-0.13	-0.69	C6H14CL1N1O2	LEUCINE HYOROCHLORIOE
1961	N-BUTANOL	295	52	-0.08	-0.62	C6H14CL1N1O2	I-LEUCINE HYOROCHLORIOE
1962	OILS	271		0.93	1.20 B	C6H14F1O3P1	OI-I-PROPYLFLUOROPHOSPHATE
1963	CCL4	228		1.57	1.47 B	C6H14F1O3P1	OI-I-PROPYLFLUOROPHOSPHATE
1964	CCL4	271		1.58	1.38 B	C6H14F1O3P1	OI-I-PROPYLFLUOROPHOSPHATE
1965	OILS	271		1.18	1.33 B	C6H14F1O3P1	OI-N-PROPYLFLUOROPHOSPHATE
1966	CCL4	271		1.78	3.20 N	C6H14F1O3P1	OI-N-PROPYLFLUOROPHOSPHATE
1967	SEC-BUTANOL	84	19	-1.66	-2.82	C6H14N2O2	LYSINE
1968	SEC-BUTANOL	84	19	-1.49	-2.59	C6H14N4O2	ARGININE
1969	OCTANOL	186		2.03	2.03 =	C6H14O1	BUTYL-ETHYLETHER
1970	OCTANOL	56		2.03	2.03 =	C6H14O1	HEXANOL
1971	OILS	201		0.88	1.99 A	C6H14O1	HEXANOL
1972	OCTANE	59		0.28		C6H14O1	HEXANOL
1973	OOOECANE	59		0.22		C6H14O1	HEXANOL
1974	HEXAOECANE	59		0.11		C6H14O1	HEXANOL
1975	OCTANOL	218		2.03	2.03 =	C6H14O1	PROPYL ETHER
1976	OILS	173		0.18	0.51 B	C6H14O2	OIETHYLACETAL
1977	OILS	224		0.90	1.17 B	C6H14O2	OIETHYLACETAL
1978	OIETHYL ETHER	3		-0.92	-0.69 A	C6H14O2	1,6-HEXANEOIOL
1979	OILS	2		-2.17	-0.74 A	C6H14O2	1,6-HEXANEOIOL
1980	OILS	2		-1.62	-0.24 A	C6H14O2	METHYLPENTANEOIOL
1981	OIETHYL ETHER	3		-0.29	-0.14 A	C6H14O2	2,4-PENTANEOIOL,2-METHYL
1982	OIETHYL ETHER	2		-1.19	-0.93 A	C6H14O3	OIETHYLENE GLYCOL MONOETHYL ETHER
1983	OILS	2		-2.22	-0.79 A	C6H14O3	OIETHYLENE GLYCOL,MONOETHYL ETHER
1984	OIETHYL ETHER	2		-1.45	-1.17 A	C6H14O3	OIPROPYLENE GLYCOL
1985	OILS	2		-2.70	-1.23 A	C6H14O3	OIPROPYLENE GLYCOL
1986	OIETHYL ETHER	2		-2.51	-2.09 A	C6H14O3	HEXANETRIOL
1987	OIETHYL ETHER	3		-2.51	-2.08 A	C6H14O4	TRIETHYLENE GLYCOL
1988	I-BUTANOL	4		-0.58	-1.32	C6H14O4	TRIETHYLENE GLYCOL
1989	I-BUTANOL	4		-1.85	-3.10	C6H14O6	MANNITOL
1990	N-BUTANOL	181	10	0.00		C6H14O12P2	HEXOSE-OIPHOSPHATE
1991	PRIM. PENTANOLS	181	10	0.23		C6H14O12P2	HEXOSE-OIPHOSPHATE
1992	HEXANOL	181	18	-0.15		C6H14O12P2	HEXOSE-OIPHOSPHATE
1993	XYLENE	46		1.17	1.84 B	C6H15N1	OI-I-PROPYLAMINE
1994	OCTANOL	218		1.70	1.70 =	C6H15N1	DIMETHYLBUTYLAMINE
1995	OCTANOL	218		1.73	1.73 =	C6H15N1	DIPROPYLAMINE
1996	OIETHYL ETHER	3		0.95	1.69 B	C6H15N1	OIPROPYLAMINE
1997	BENZENE	205		1.05	1.28 B	C6H15N1	OIPROPYLAMINE
1998	1-BUTANOL	4		1.62	1.77	C6H15N1	OIPROPYLAMINE
1999	XYLENE	46		1.24	1.87 B	C6H15N1	OIPROPYLAMINE
2000	TOLUENE	68		1.16	1.47 B	C6H15N1	OIPROPYLAMINE

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2001	I-BUTANOL	4		2.02	2.34	C6H15N1	HEXYLAMINE
2002	XYLENE	46		0.89	1.52 B	C6H15N1	HEXYLAMINE
2003	OCTANOL	218		1.44	1.44 =	C6H15N1	TRIETHYLAMINE
2004	BENZENE	355		1.13	1.30 B	C6H15N1	TRIETHYLAMINE
2005	I-BUTANOL	4		1.32	1.47	C6H15N1	TRIETHYLAMINE
2006	XYLENE	46		1.11	1.77 B	C6H15N1	TRIETHYLAMINE
2007	TOLUENE	68		1.00	1.37 B	C6H15N1	TRIETHYLAMINE
2008	TOLUENE	66		0.76	1.20 B	C6H15N1	TRIETHYLAMINE
2009	TOLUENE	355		0.92	1.32 B	C6H15N1	TRIETHYLAMINE
2010	PRIM. PENTANOLS	182		1.42	1.42	C6H15N1	TRIETHYLAMINE
2011	DIETHYL ETHER	3		-0.46	0.46 B	C6H15N1O1	DIETHYLETHANOLAMINE
2012	I-BUTANOL	4		0.58	0.31	C6H15N1O1	DIETHYLETHANOLAMINE
2013	OCTANOL	5		-0.82	-0.82 =	C6H15N1O2	DI-I-PROPANOLAMINE
2014	DIETHYL ETHER	3		-2.23	-1.10 B	C6H15N1O2	DI-I-PROPANOLAMINE
2015	I-BUTANOL	4		-0.15	-0.72	C6H15N1O2	DI-I-PROPANOLAMINE
2016	DIETHYL ETHER	3		-2.96	-1.75 B	C6H15N1O3	TRIETHANOLAMINE
2017	I-BUTANOL	4		-0.58	-1.32	C6H15N1O3	TRIETHANOLAMINE
2018	CCL4	135		1.90	1.67 B	C6H15O2P1S2	PHOSPHORODITHIOTIC ACID,DI-I-PROPYL
2019	PRIM. PENTANOLS	236	17	0.73	0.62	C6H15O4P1	PHOSPHATE,DI-N-PROPYL
2020	OCTANOL	56		0.30	0.30 =	C6H16N2	ETHYLENEDIAMINE, N,N,N',N'-TETRAMETHYL
2021	OCTANOL	298		3.57	3.57 =	C6H16SI1	SILANE, BUTYL-DIMETHYL
2022	OCTANOL	298		3.84	3.84 =	C6H16SI1	SILANE, PROPYL-TRIMETHYL
2023	OCTANOL	56		0.28	0.28 =	C6H18N3O1P1	HEXAMETHYL PHOSPHORIC TRIAMIDE
2024	I-BUTANOL	4		-0.82	-1.66	C6H18N4	TRIETHYLENETETRAMINE
2025	OCTANOL	206		4.53	4.53 =	C7H1CL5N2	BENZIMIDAZOLE,2,4,5,6,7-PENTACHLORO-
2026	OCTANOL	206	27	3.50	3.50 =	C7H2CL2F3N3	4-PYRIDINE IMIDAZOLE,2-TRIFLOROME-6,7-DICL
2027	HEXANE	299		0.49		C7H3BR2N1O1	4-HYDROXY-3,5-DIBROMOBENZONITRILE
2028	OCTANOL	206	27	2.69	2.69 =	C7H3CL1F3N3	4-PYRIDINE IMIDAZOLE,2-TRIFLUOROME-6-CL
2029	HEXANE	299		-0.14		C7H3CL2N1O1	4-HYDROXY-3,5-DICHLOROBENZONITRILE
2030	HEXANE	299		1.08		C7H3I2N1O1	4-HYDROXY-3,5-DIIODOBENZONITRILE
2031	DIETHYL ETHER	46		0.27	0.36 A	C7H3N3O8	2,4,6-TRINITROBENZOIC ACID
2032	OILS	173		2.61	3.56 A	C7H4BR1N1	BROMOBENZONITRILE
2033	OCTANOL	206	27	1.23	1.23 =	C7H4F3N3	4-PYRIDINE IMIDAZOLE,2-TRIFLUOROMETHYL
2034	OCTANOL	206	27	0.94	0.94 =	C7H4F3N3	5-PYRIDINE IMIDAZOLE,2-TRIFLUOROMETHYL
2035	OCTANOL	10		1.17	1.17 =	C7H4N2O2	BENZENE,3-CYANO-1-NITRO
2036	OCTANOL	10		1.19	1.19 =	C7H4N2O2	BENZENE,4-CYANO-1-NITRO
2037	DIETHYL ETHER	46		1.18	1.16 A	C7H4N2O6	2,4-DINITROBENZOIC ACID
2038	CHCL3	46		-0.88	0.42 A	C7H4N2O6	2,4-DINITROBENZOIC ACID
2039	XYLENE	46		-0.92	0.79 A	C7H4N2O6	2,4-DINITROBENZOIC ACID
2040	CHCL3	149		0.18	1.38 A	C7H4N2O6	3,5-DINITROBENZOIC ACID
2041	CHCL3	46		0.07	1.28 A	C7H4N2O6	3,5-DINITROBENZOIC ACID
2042	CHCL3	356		-0.20	1.04 A	C7H4N2O6	3,5-DINITROBENZOIC ACID
2043	XYLENE	46		0.09	1.90 A	C7H4N2O6	3,5-DINITROBENZOIC ACID
2044	ME-I-BUT.KETONE	149		2.48	2.22	C7H4N2O6	3,5-DINITROBENZOIC ACID
2045	OCTANOL	276		1.60	1.60 =	C7H4N4O4	5,7-DINITROBENZPYRAZOLE /PKA = 1.20/
2046	OCTANOL	10		2.87	2.87 =	C7H5BR1O2	M-BROMOBENZOIC ACID
2047	CHCL3	29		2.04	3.07 A	C7H5BR1O2	M-BROMOBENZOIC ACID
2048	CHCL3	29		0.91	2.05 A	C7H5BR1O2	O-BROMOBENZOIC ACID
2049	OCTANOL	10		2.86	2.86 =	C7H5BR1O2	P-BROMOBENZOIC ACID
2050	OCTANOL	218		2.46	2.46 =	C7H5CL1N2O1	BENZOXAZOLE,2-AMINO-5-CHLORO/ZOXAZOLAMINE/
2051	OCTANOL	10		2.68	2.68 =	C7H5CL1O2	M-CHLOROBENZOIC ACID
2052	CHCL3	29	12	1.92	3.05 A	C7H5CL1O2	M-CHLOROBENZOIC ACID
2053	TOLUENE	29		1.12	2.56 A	C7H5CL1O2	M-CHLOROBENZOIC ACID
2054	OCTANOL	65		1.98	1.98 =	C7H5CL1O2	O-CHLOROBENZOIC ACID
2055	DIETHYL ETHER	46		2.14	2.00 A	C7H5CL1O2	O-CHLOROBENZOIC ACID
2056	CYCLOHEXANE	357		-0.34		C7H5CL1O2	O-CHLOROBENZOIC ACID
2057	CHCL3	29		0.90	2.03 A	C7H5CL1O2	O-CHLOROBENZOIC ACID
2058	XYLENE	46		0.01	1.80 A	C7H5CL1O2	O-CHLOROBENZOIC ACID
2059	TOLUENE	29		0.27	1.81 A	C7H5CL1O2	O-CHLOROBENZOIC ACID
2060	OCTANOL	10		2.65	2.65 =	C7H5CL1O2	P-CHLOROBENZOIC ACID
2061	CHCL3	29		1.72	2.78 A	C7H5CL1O2	P-CHLOROBENZOIC ACID
2062	TOLUENE	29		1.26	2.68 A	C7H5CL1O2	P-CHLOROBENZOIC ACID
2063	OCTANOL	235		2.92	2.92 =	C7H5CL3	A,A,A-TRICHLOROTOLUENE
2064	OCTANOL	10		2.15	2.15 =	C7H5F1O2	M-FLUOROBENZOIC ACID
2065	OCTANOL	10		2.07	2.07 =	C7H5F1O2	P-FLUOROBENZOIC ACID
2066	OCTANOL	56		2.79	2.79 =	C7H5F3	BENZENE, TRIFLUOROMETHYL
2067	OCTANOL	217	07	1.73	1.73 =	C7H5F3N2O4S1	3-TRICHLOROMETHYL-4-NITROBENZENESULFONAMIDE
2068	CHCL3	217	07	0.19	1.44 A	C7H5F3N2O4S1	3-TRICHLOROMETHYL-4-NITROBENZENESULFONAMIDE
2069	OCTANOL	56		3.17	3.17 =	C7H5F3O1	BENZENE, TRIFLUOROMETHOXY
2070	OCTANOL	10		2.95	2.95 =	C7H5F3O1	M-TRIFLUOROMETHYLPHENOL
2071	OCTANOL	261		2.80	2.80 =	C7H5F3O1	O-TRIFLUOROMETHYLPHENOL
2072	OCTANOL	56		2.71	2.71 =	C7H5F3O2S1	SULFONE,PHENYL-TRIFLUOROMETHYL
2073	OCTANOL	56		3.79	3.79 =	C7H5F3S1	BENZENE, TRIFLUOROMETHYLTHIO
2074	OCTANOL	10		3.13	3.13 =	C7H5I1O2	M-IODOBENZOIC ACID
2075	OCTANOL	65		2.40	2.40 =	C7H5I1O2	O-IODOBENZOIC ACID
2076	DIETHYL ETHER	46		3.11	2.85 A	C7H5I1O2	O-IODOBENZOIC ACID
2077	CHCL3	46		1.09	2.21 A	C7H5I1O2	O-IODOBENZOIC ACID
2078	XYLENE	46		0.49	2.32 A	C7H5I1O2	O-IODOBENZOIC ACID
2079	OCTANOL	10		3.02	3.02 =	C7H5I1O2	P-IODOBENZOIC ACID
2080	OCTANOL	10		1.56	1.56 =	C7H5N1	BENZONITRILE
2081	CYCLOHEXANE	358		1.06		C7H5N1	BENZONITRILE
2082	OCTANOL	309		1.59	1.59 =	C7H5N1O1	BENZOXAZOLE
2083	OCTANOL	10		1.70	1.70 =	C7H5N1O1	M-CYANOPHENOL
2084	OCTANOL	10		1.60	1.60 =	C7H5N1O1	P-CYANOPHENOL
2085	DIETHYL ETHER	112		1.79	1.68 A	C7H5N1O1S1	BENZOXAZOLTHION
2086	OCTANOL	65		0.91	0.91 =	C7H5N1O3S1	SACCHARIN
2087	DIETHYL ETHER	359	16	0.64	0.67 A	C7H5N1O3S1	SACCHARIN
2088	DIETHYL ETHER	113	16	0.60	0.64 A	C7H5N1O3S1	SACCHARIN
2089	CHCL3	113	16	-0.06	1.17 A	C7H5N1O3S1	SACCHARIN
2090	1-PENT. ACETATE	359	12	1.51	1.39	C7H5N1O3S1	SACCHARIN
2091	OCTANOL	10		1.83	1.83 =	C7H5N1O4	M-NITROBENZOIC ACID
2092	DIETHYL ETHER	46		1.97	1.85 A	C7H5N1O4	M-NITROBENZOIC ACID
2093	CHCL3	29		0.48	1.66 A	C7H5N1O4	M-NITROBENZOIC ACID
2094	CHCL3	254		0.41	1.55 A	C7H5N1O4	M-NITROBENZOIC ACID
2095	BENZENE	356		0.21	1.58 A	C7H5N1O4	M-NITROBENZOIC ACID
2096	XYLENE	46		0.02	1.83 A	C7H5N1O4	M-NITROBENZOIC ACID
2097	TOLUENE	29		0.09	1.66 A	C7H5N1O4	M-NITROBENZOIC ACID
2098	N-HEPTANE	254		-1.22		C7H5N1O4	M-NITROBENZOIC ACID
2099	DIETHYL ETHER	46		1.59	1.52 A	C7H5N1O4	O-NITROBENZOIC ACID
2100	CYCLOHEXANE	357		-0.88		C7H5N1O4	O-NITROBENZOIC ACID

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2101	CHCL3	29		0.03	1.25 A	C7H5N1O4	O-NITROBENZOIC ACID
2102	CHCL3	46		-0.19	1.04 A	C7H5N1O4	O-NITROBENZOIC ACID
2103	BENZENE	307		-0.30	1.12 A	C7H5N1O4	O-NITROBENZOIC ACID
2104	BENZENE	356		-0.21	1.16 A	C7H5N1O4	O-NITROBENZOIC ACID
2105	XYLENE	46		-0.35	1.31 A	C7H5N1O4	O-NITROBENZOIC ACID
2106	TOLUENE	29		-0.32	1.30 A	C7H5N1O4	O-NITROBENZOIC ACID
2107	OCTANOL	10		1.89	1.89 =	C7H5N1O4	P-NITROBENZOIC ACID
2108	CHCL3	29		0.86	2.00 A	C7H5N1O4	P-NITROBENZOIC ACID
2109	BENZENE	307		0.31	1.67 A	C7H5N1O4	P-NITROBENZOIC ACID
2110	XYLENE	46		0.07	1.85 A	C7H5N1O4	P-NITROBENZOIC ACID
2111	TOLUENE	29		0.51	2.03 A	C7H5N1O4	P-NITROBENZOIC ACID
2112	OCTANOL	186		2.01	2.01 =	C7H5N1S1	BENZOTHIAZOLE
2113	OCTANOL	309		2.03	2.03 =	C7H5N1S1	BENZOTHIAZOLE
2114	OCTANOL	218		3.28	3.28 =	C7H5N1S1	PHENYLISOTHIOCYANATE
2115	OCTANOL	238		3.22	3.22 =	C7H5N1S1	PHENYLISOTHIOCYANATE
2116	OCTANOL	206		1.64	1.64 =	C7H5N3O2	BENZIMIDAZOLE,5-NITRO
2117	OCTANOL	216	78	-0.85	-0.85 =	C7H5NA1O3	SODIUM SALICYLATE
2118	OILS	292		-0.97	-0.37 B	C7H5NA1O3	SODIUM SALICYLATE
2119	BENZENE	311	6	0.35		C7H6B1F3O2	PHENYLBORONIC ACID,3-TRIFLUOROMETHYL
2120	BENZENE	311	6	-1.71		C7H6B1N1O6	PHENYLBORONIC ACID,3-NITRO,4-CARBOXYL
2121	OCTANOL	206		2.39	2.39 =	C7H6CL1N3S1	4-PYRIDINE IMIDAZOLE,2-METHYLTHIO-6-CHLORO
2122	OCTANOL	216		1.82	1.82 =	C7H6N2	7-AZAINDOLE
2123	OCTANOL	218		1.34	1.34 =	C7H6N2	BENZIMIDAZOLE
2124	OCTANOL	206		1.50	1.50 =	C7H6N2	BENZIMIDAZOLE
2125	OCTANOL	360		1.20	1.20 =	C7H6N2	BENZIMIDAZOLE
2126	DIETHYL ETHER	112		-0.02	0.82 B	C7H6N2	BENZIMIDAZOLE
2127	CHCL3	112	50	-0.10	1.12 A	C7H6N2	BENZIMIDAZOLE
2128	OCTANOL	309		1.82	1.82 =	C7H6N2	INDAZOLE
2129	OCTANOL	217	07	0.23	0.23 =	C7H6N2O2S1	P-CYANOBENZENESULFONAMIDE
2130	CHCL3	217	07	-0.61	0.01 N	C7H6N2O2S1	P-CYANOBENZENESULFONAMIDE
2131	OCTANOL	235		1.48	1.48 =	C7H6O1	BENZALDEHYDE
2132	DIETHYL ETHER	248	50	1.74	2.41 B	C7H6O1	BENZALDEHYDE
2133	CYCLOHEXANE	141		1.13		C7H6O1	BENZALDEHYDE
2134	CYCLOHEXANE	248		1.34		C7H6O1	BENZALDEHYDE
2135	BENZENE	248	50	2.10	2.00 B	C7H6O1	BENZALDEHYDE
2136	CLCH2CH2CL	248		2.35		C7H6O1	BENZALDEHYDE
2137	OCTANOL	10		1.87	1.87 =	C7H6O2	BENZOIC ACID
2138	DIETHYL ETHER	3		1.89	1.78 A	C7H6O2	BENZOIC ACID
2139	DIETHYL ETHER	46		1.78	1.68 A	C7H6O2	BENZOIC ACID
2140	DIETHYL ETHER	36		1.85	1.72 A	C7H6O2	BENZOIC ACID
2141	CHCL3	29		0.71	1.86 A	C7H6O2	BENZOIC ACID
2142	CHCL3	39		0.30	1.51 A	C7H6O2	BENZOIC ACID
2143	CHCL3	254		0.46	1.60 A	C7H6O2	BENZOIC ACID
2144	CHCL3	17		0.54	1.73 A	C7H6O2	BENZOIC ACID
2145	OILS	361		0.66	1.86 A	C7H6O2	BENZOIC ACID
2146	OILS	362		0.54	1.71 A	C7H6O2	BENZOIC ACID
2147	BENZENE	29		0.21	1.58 A	C7H6O2	BENZOIC ACID
2148	BENZENE	39		0.24	1.61 A	C7H6O2	BENZOIC ACID
2149	BENZENE	38		0.18	1.55 A	C7H6O2	BENZOIC ACID
2150	BENZENE	363	12	-0.21	1.17 A	C7H6O2	BENZOIC ACID
2151	BENZENE	36		0.36	1.73 A	C7H6O2	BENZOIC ACID
2152	BENZENE	20		0.12	1.49 A	C7H6O2	BENZOIC ACID
2153	1-BUTANOL	4		1.69	1.87	C7H6O2	BENZOIC ACID
2154	XYLENE	46		-0.19	1.58 A	C7H6O2	BENZOIC ACID
2155	XYLENE	36	12	0.44	2.23 A	C7H6O2	BENZOIC ACID
2156	TOLUENE	29		0.36	1.90 A	C7H6O2	BENZOIC ACID
2157	TOLUENE	36		0.48	2.00 A	C7H6O2	BENZOIC ACID
2158	CCL4	364	12	-2.90		C7H6O2	BENZOIC ACID
2159	ETHYL BENZOATE	17		1.50		C7H6O2	BENZOIC ACID
2160	DI-PENTYL ETHER	17		0.95		C7H6O2	BENZOIC ACID
2161	N-HEPTANE	254		-0.72		C7H6O2	BENZOIC ACID
2162	PARAFFINS	291		-0.12		C7H6O2	BENZOIC ACID
2163	DIETHYL ETHER	248		1.32	1.27 A	C7H6O2	M-HYDROXYBENZALDEHYDE
2164	BENZENE	248		-0.16	1.21 A	C7H6O2	M-HYDROXYBENZALDEHYDE
2165	CLCH2CH2CL	248		0.44		C7H6O2	M-HYDROXYBENZALDEHYDE
2166	OCTANOL	365		1.70	1.70 =	C7H6O2	O-HYDROXYBENZALDEHYDE/SALICYLALDEHYDE/
2167	OCTANOL	268	32	1.81	1.81 =	C7H6O2	O-HYDROXYBENZALDEHYDE/SALICYLALDEHYDE/
2168	TOLUENE	150		2.15	2.70 B	C7H6O2	O-HYDROXYBENZALDEHYDE/SALICYLALDEHYDE/
2169	DIETHYL ETHER	366		1.10	1.08 A	C7H6O2	P-HYDROXYBENZALDEHYDE
2170	CHCL3	366		-0.12	1.11 A	C7H6O2	P-HYDROXYBENZALDEHYDE
2171	BENZENE	366		-0.55	0.87 A	C7H6O2	P-HYDROXYBENZALDEHYDE
2172	CCL4	366		-1.70	0.41 A	C7H6O2	P-HYDROXYBENZALDEHYDE
2173	CLCH2CH2CL	366		0.11		C7H6O2	P-HYDROXYBENZALDEHYDE
2174	CLCH2CH2CL	248		0.21		C7H6O2	P-HYDROXYBENZALDEHYDE
2175	DI-I-PR. ETHER	366		0.84	1.51	C7H6O2	P-HYDROXYBENZALDEHYDE
2176	OCTANOL	9		0.53	0.53 =	C7H6O2	TROPOLONE
2177	CHCL3	367	12	1.70	1.21 B	C7H6O2	TROPOLONE
2178	OCTANOL	10		1.50	1.50 =	C7H6O3	M-HYDROXYBENZOIC ACID
2179	DIETHYL ETHER	3		1.32	1.27 A	C7H6O3	M-HYDROXYBENZOIC ACID
2180	I-BUTANOL	4		1.40	1.47	C7H6O3	M-HYDROXYBENZOIC ACID
2181	OCTANOL	186		2.26	2.26 =	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2182	OCTANOL	218		2.21	2.21 =	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2183	DIETHYL ETHER	3		2.37	2.20 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2184	DIETHYL ETHER	46		2.53	2.32 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2185	CYCLOHEXANE	15		-1.02		C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2186	CYCLOHEXANE	357		-0.50		C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2187	CHCL3	149		0.48	1.66 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2188	CHCL3	29		0.50	1.67 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2189	CHCL3	39	12	0.34	1.46 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2190	CHCL3	254		0.46	1.60 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2191	OILS	173		1.00	2.10 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2192	BENZENE	39		0.45	1.81 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2193	BENZENE	368	68	0.38	1.88 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2194	I-BUTANOL	4		2.13	2.31	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2195	XYLENE	46		0.11	1.93 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2196	TOLUENE	29		0.31	1.80 A	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2197	CCL4	17		-0.30		C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2198	ETHYL BENZOATE	17		1.90		C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2199	N-HEPTANE	254		-0.92		C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/
2200	ME-I-BUT.KETONE	149		2.51	2.25	C7H6O3	O-HYDROXYBENZOIC ACID/SALICYLIC ACID/

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2201	OCTANOL	10		1.58	1.58 =	C7H6O3	P-HYDROXYBENZOIC ACID
2202	DIETHYL ETHER	3		1.42	1.36 A	C7H6O3	P-HYDROXYBENZOIC ACID
2203	DIETHYL ETHER	46		1.00	1.00 A	C7H6O3	P-HYDROXYBENZOIC ACID
2204	CHCL3	254	12	-2.00	-0.59 A	C7H6O3	P-HYDROXYBENZOIC ACID
2205	OILS	369		0.22	1.45 A	C7H6O3	P-HYDROXYBENZOIC ACID
2206	I-BUTANOL	4		1.43	1.51	C7H6O3	P-HYDROXYBENZOIC ACID
2207	ETHYL BENZOATE	17		0.75		C7H6O3	P-HYDROXYBENZOIC ACID
2208	DI-PENTYL ETHER	17		-0.39		C7H6O3	P-HYDROXYBENZOIC ACID
2209	XYLENE	46	12	-1.66	-0.02 A	C7H6O4	2,4-DIHYDROXYBENZOIC ACID/RESORCYLIC ACID/
2210	ME-I-BUT.KETONE	195		1.55	1.44	C7H6O4	2,4-DIHYDROXYBENZOIC ACID /RESORCYLIC ACID/
2211	DIETHYL ETHER	46		1.35	1.31 A	C7H6O4	2,5-DIHYDROXYBENZOIC ACID/GENTISIC ACID/
2212	CHCL3	46	12	-1.57	-0.21 A	C7H6O4	2,5-DIHYDROXYBENZOIC ACID/GENTISIC ACID/
2213	XYLENE	46	12	-1.82	-0.20 A	C7H6O4	2,5-DIHYDROXYBENZOIC ACID/GENTISIC ACID/
2214	OCTANOL	56		2.20	2.20 =	C7H6O4	2,6-DIHYDROXYBENZOIC ACID
2215	DIETHYL ETHER	46		1.45	1.39 A	C7H6O4	3,5-DIHYDROXYBENZOIC ACID
2216	DIETHYL ETHER	3		-0.30	-0.15 A	C7H6O5	3,4,5-TRIHYDROXYBENZOIC ACID/GALLIC ACID/
2217	DIETHYL ETHER	46		-0.42	-0.25 A	C7H6O5	3,4,5-TRIHYDROXYBENZOIC ACID/GALLIC ACID/
2218	DIETHYL ETHER	207		-1.56	-1.25 A	C7H6O6S1	SULFOSALICYLIC ACID/3-CO2H-4-OH-BENZENESULFONIC ACID/
2219	ME-I-BUT.KETONE	195		-1.25	-1.17	C7H6O6S1	SULFOSALICYLIC ACID/3-CO2H-4-OH-BENZENESULFONIC ACID/
2220	S-PENTANOLS	195		-1.08	-1.54	C7H6O6S1	SULFOSALICYLIC ACID/3-CO2H-4-OH-BENZENESULFONIC ACID/
2221	BENZENE	311	6	-1.46		C7H7B1O3	P-FORMYLPHENYLBORONIC ACID
2222	BENZENE	311	6	-2.52		C7H7B1O4	M-CARBOXYPHENYLBORONIC ACID
2223	BENZENE	311	6	-1.83		C7H7B1O4	P-CARBOXYPHENYLBORONIC ACID
2224	OCTANOL	218	26	2.92	2.92 =	C7H7BR1	A-BROMOTOLUENE
2225	OCTANOL	302		2.30	2.30 =	C7H7CL1	A-CHLOROTOLUENE
2226	OCTANOL	301		3.28	3.28 =	C7H7CL1	M-CHLOROTOLUENE
2227	OCTANOL	301		3.42	3.42 =	C7H7CL1	O-CHLOROTOLUENE
2228	OCTANOL	301		3.33	3.33 =	C7H7CL1	P-CHLOROTOLUENE
2229	OCTANOL	206	27	3.70	3.70 =	C7H7CL1N4O4S2	PURINE,2,6-DI-(METHYLSULFONYL)-8-CHLORO
2230	OCTANOL	206		0.63	0.63 =	C7H7CL1N4S2	PURINE,2,8-DIMETHYLTHIO,6-CHLORO
2231	OCTANOL	10		1.94	1.94 =	C7H7CL1O1	M-CHLOROBENZYL ALCOHOL
2232	OCTANOL	10		1.96	1.96 =	C7H7CL1O1	P-CHLOROBENZYL ALCOHOL
2233	OCTANOL	261		3.10	3.10 =	C7H7CL1O1	PHENOL,4-CHLORO,3-METHYL
2234	CYCLOHEXANE	124		0.15		C7H7CL1O1	PHENOL,4-CHLORO,3-METHYL
2235	METH. DECANOATE	124		2.65	3.14	C7H7CL1O1	PHENOL,4-CHLORO,3-METHYL
2236	OLEYL ALCOHOL	124		2.46	3.00	C7H7CL1O1	PHENOL,4-CHLORO,3-METHYL
2237	OCTANOL	65		2.74	2.74 =	C7H7F1O2S1	P-FLUOROSULFONYLTOLUENE
2238	1-OCTANOL	353		-2.83		C7H7K1O2	POTASSIUM GUAICOLATE
2239	OCTANOL	235		1.75	1.75 =	C7H7N1O1	BENZALDOXIME
2240	OCTANOL	10		0.64	0.64 =	C7H7N1O1	BENZAMIDE
2241	DIETHYL ETHER	248		-0.22	0.65 B	C7H7N1O1	BENZAMIDE
2242	CHCL3	248		0.11	0.71 N	C7H7N1O1	BENZAMIDE
2243	OILS	173		-0.51	0.73 A	C7H7N1O1	BENZAMIDE
2244	OILS	82		-0.36	0.87 A	C7H7N1O1	BENZAMIDE
2245	OILS	293		-0.66	0.59 A	C7H7N1O1	BENZAMIDE
2246	OILS	249		-0.42	0.81 A	C7H7N1O1	BENZAMIDE
2247	OILS	70		-0.36	0.89 A	C7H7N1O1	BENZAMIDE
2248	BENZENE	248		-0.71	0.68 A	C7H7N1O1	BENZAMIDE
2249	CCL4	248		-1.54		C7H7N1O1	BENZAMIDE
2250	CLCH2CH2CL	248		0.00		C7H7N1O1	BENZAMIDE
2251	OLEYL ALCOHOL	82		0.40	0.96	C7H7N1O1	BENZAMIDE
2252	OCTANOL	56		1.15	1.15 =	C7H7N1O1	FORMANILIDE
2253	DIETHYL ETHER	3		0.18	0.27 A	C7H7N1O2	M-AMINOBENZOIC ACID
2254	1-BUTANOL	4		0.46	0.14	C7H7N1O2	M-AMINOBENZOIC ACID
2255	OCTANOL	56		1.21	1.21 =	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2256	DIETHYL ETHER	3		1.43	1.37 A	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2257	DIETHYL ETHER	112		1.48	1.41 A	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2258	DIETHYL ETHER	46	12	0.05	0.17 A	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2259	CHCL3	112	12	0.57	1.73 A	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2260	CHCL3	29	25	-1.15	0.27 A	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2261	BENZENE	72		-0.27	1.11 A	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2262	1-BUTANOL	4		1.18	1.15	C7H7N1O2	O-AMINOBENZOIC ACID/ANTHRANILIC ACID/
2263	OCTANOL	65		0.68	0.68 =	C7H7N1O2	P-AMINOBENZOIC ACID
2264	DIETHYL ETHER	3		0.88	0.89 A	C7H7N1O2	P-AMINOBENZOIC ACID
2265	1-BUTANOL	4		0.89	0.75	C7H7N1O2	P-AMINOBENZOIC ACID
2266	OCTANOL	186		1.28	1.28 =	C7H7N1O2	O-HYDROXYBENZAMIDE/SALICYLAMIDE/
2267	OILS	173		0.45	1.60 A	C7H7N1O2	O-HYDROXYBENZAMIDE/SALICYLAMIDE/
2268	OILS	224	12	1.15		C7H7N1O2	O-HYDROXYBENZAMIDE/SALICYLAMIDE/
2269	OILS	82		0.41	1.56 A	C7H7N1O2	O-HYDROXYBENZAMIDE/SALICYLAMIDE/
2270	OILS	293		0.34	1.50 A	C7H7N1O2	O-HYDROXYBENZAMIDE/SALICYLAMIDE/
2271	OILS	70	12	1.15	2.23 A	C7H7N1O2	O-HYDROXYBENZAMIDE/SALICYLAMIDE/
2272	OLEYL ALCOHOL	82		0.77	1.33	C7H7N1O2	O-HYDROXYBENZAMIDE /SALICYLAMIDE/
2273	CHCL3	318		2.01	1.49 B	C7H7N1O2	1-NICOTINIC ACID,METHYL ESTER
2274	OCTANOL	10		2.45	2.45 =	C7H7N1O2	M-NITROTOLUENE
2275	OCTANOL	301		2.40	2.40 =	C7H7N1O2	M-NITROTOLUENE
2276	OCTANOL	301		2.30	2.30 =	C7H7N1O2	O-NITROTOLUENE
2277	OCTANOL	10		2.37	2.37 =	C7H7N1O2	P-NITROTOLUENE
2278	OCTANOL	301		2.42	2.42 =	C7H7N1O2	P-NITROTOLUENE
2279	OCTANOL	56		1.08	1.08 =	C7H7N1O2	O-PHENYL CARBAMATE
2280	N-HEPTANE	370	14	-1.04		C7H7N1O3	P-AMINOSALICYLIC ACID
2281	OCTANOL	10		2.16	2.16 =	C7H7N1O3	M-NITROANISOLE
2282	OCTANOL	10		2.03	2.03 =	C7H7N1O3	P-NITROANISOLE
2283	OCTANOL	10		1.21	1.21 =	C7H7N1O3	M-NITROBENZYL ALCOHOL
2284	OCTANOL	10		1.26	1.26 =	C7H7N1O3	P-NITROBENZYL ALCOHOL
2285	I-OCTANOL	353		-2.62		C7H7NA1O2	SODIUM GUAICOLATE
2286	OCTANOL	10		2.69	2.69 =	C7H8	TOLUENE
2287	OCTANOL	56		2.73	2.73 =	C7H8	TOLUENE
2288	OCTANOL	309		2.11	2.11 =	C7H8	TOLUENE
2289	OCTANOL	301		2.80	2.80 =	C7H8	TOLUENE
2290	N-HEPTANE	310		2.85		C7H8	TOLUENE
2291	OCTANOL	218		-0.07	-0.07 =	C7H8CL1N3O4S2	HYDROCHLOROTHIAZIDE
2292	BENZENE	72		0.51	0.91 B	C7H8N2O1	P-NITROSOMETHYLANILINE
2293	OCTANOL	56		0.83	0.83 =	C7H8N2O1	PHENYLUREA
2294	OCTANOL	235		0.82	0.82 =	C7H8N2O1	PHENYLUREA
2295	DIETHYL ETHER	3		0.04	0.81 B	C7H8N2O1	PHENYLUREA
2296	DIETHYL ETHER	113		-0.26	-0.10 A	C7H8N2O1	PHENYLUREA
2297	CHCL3	113	12	-0.72	-0.07 N	C7H8N2O1	PHENYLUREA
2298	OCTANOL	235		0.73	0.73 =	C7H8N2S1	PHENYLTHIOUREA
2299	DIETHYL ETHER	248		0.23	0.32 A	C7H8N2S1	PHENYLTHIOUREA
2300	CHCL3	248		0.54	1.10 N	C7H8N2S1	PHENYLTHIOUREA

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2301	OCTANOL	226		1.04	1.04 =	C7H8N4O1S1	5-HYDROXYPICOLINALDEHYDE THIOSEMICARBAZONE(107392)
2302	OCTANOL	65		1.04	1.04 =	C7H8N4O1S1	5-HYDROXYPICOLINALDEHYDE THIOSEMICARBAZONE(107392)
2303	OCTANOL	218		-0.78	-0.78 =	C7H8N4O2	THEOBROMINE/3,7-DIMETHYLXANTHINE/
2304	CHCL3	254		-0.40	-0.45 B	C7H8N4O2	THEOBROMINE/3,7-DIMETHYLXANTHINE/
2305	CHCL3	322		-0.91	-0.85 B	C7H8N4O2	THEOBROMINE/3,7-DIMETHYLXANTHINE/
2306	OILS	371	12	0.19	1.36 A	C7H8N4O2	THEOBROMINE/3,7-DIMETHYLXANTHINE/
2307	OCTANOL	218		-0.02	-0.02 =	C7H8N4O2	THEOPHYLLINE/1,3-DIMETHYLXANTHINE/
2308	CHCL3	254		-0.52	-0.54 B	C7H8N4O2	THEOPHYLLINE/1,3-DIMETHYLXANTHINE/
2309	CHCL3	322	12	-0.86	-0.80 B	C7H8N4O2	THEOPHYLLINE/1,3-DIMETHYLXANTHINE/
2310	OILS	371	12	0.21	0.46 B	C7H8N4O2	THEOPHYLLINE/1,3-DIMETHYLXANTHINE/
2311	CCL4	234	12	-2.70		C7H8N4O2	THEOPHYLLINE/1,3-DIMETHYLXANTHINE/
2312	N-HEPTANE	254		-1.70		C7H8N4O2	THEOPHYLLINE/1,3-DIMETHYLXANTHINE/
2313	OCTANOL	10		2.11	2.11 =	C7H8O1	ANISOLE
2314	OCTANOL	309		2.04	2.04 =	C7H8O1	ANISOLE
2315	DIETHYL ETHER	323	50	2.46	2.27 A	C7H8O1	ANISOLE
2316	CYCLOHEXANE	358		2.30		C7H8O1	ANISOLE
2317	OCTANOL	10		1.10	1.10 =	C7H8O1	BENZYL ALCOHOL
2318	CYCLOHEXANE	141		-0.62		C7H8O1	BENZYL ALCOHOL
2319	HEXANE	372		-0.76		C7H8O1	BENZYL ALCOHOL
2320	OCTANOL	10		1.96	1.96 =	C7H8O1	M-METHYLPHENOL/CRESOL/
2321	OCTANOL	301		2.01	2.01 =	C7H8O1	M-METHYLPHENOL/CRESOL/
2322	DIETHYL ETHER	329		1.80	1.70 A	C7H8O1	M-METHYLPHENOL/CRESOL/
2323	CYCLOHEXANE	124		-0.30		C7H8O1	M-METHYLPHENOL/CRESOL/
2324	CYCLOHEXANE	132		-0.15		C7H8O1	M-METHYLPHENOL/CRESOL/
2325	CYCLOHEXANE	325		-0.20		C7H8O1	M-METHYLPHENOL/CRESOL/
2326	CYCLOHEXANE	133		-0.10		C7H8O1	M-METHYLPHENOL/CRESOL/
2327	OILS	324		1.29	2.37 A	C7H8O1	M-METHYLPHENOL/CRESOL/
2328	OILS	327		1.21	2.28 A	C7H8O1	M-METHYLPHENOL/CRESOL/
2329	BENZENE	324	45	0.88	2.24 A	C7H8O1	M-METHYLPHENOL/CRESOL/
2330	N-BUTYL ACETATE	331		2.19	1.98	C7H8O1	M-METHYLPHENOL/CRESOL/
2331	METH. DECANOATE	124		1.83	2.29	C7H8O1	M-METHYLPHENOL/CRESOL/
2332	N-HEPTANE	310		-0.35		C7H8O1	M-METHYLPHENOL/CRESOL/
2333	OLEYL ALCOHOL	124		1.79	2.34	C7H8O1	M-METHYLPHENOL/CRESOL/
2334	PARAFFINS	327		-0.51		C7H8O1	M-METHYLPHENOL/CRESOL/
2335	OCTANOL	216		1.95	1.95 =	C7H8O1	O-METHYLPHENOL
2336	CYCLOHEXANE	124		0.04		C7H8O1	O-METHYLPHENOL
2337	CYCLOHEXANE	132		0.13		C7H8O1	O-METHYLPHENOL
2338	CYCLOHEXANE	325		0.10		C7H8O1	O-METHYLPHENOL
2339	CYCLOHEXANE	133		0.20		C7H8O1	O-METHYLPHENOL
2340	OILS	327		1.34	2.49 A	C7H8O1	O-METHYLPHENOL
2341	N-BUTYL ACETATE	331		2.20	1.98	C7H8O1	O-METHYLPHENOL
2342	METH. DECANOATE	124		1.93	2.40	C7H8O1	O-METHYLPHENOL
2343	N-HEPTANE	310		-0.05		C7H8O1	O-METHYLPHENOL
2344	OLEYL ALCOHOL	124		1.81	2.36	C7H8O1	O-METHYLPHENOL
2345	PARAFFINS	327		-0.14		C7H8O1	O-METHYLPHENOL
2346	OCTANOL	10		1.94	1.94 =	C7H8O1	P-METHYLPHENOL
2347	OCTANOL	301		1.92	1.92 =	C7H8O1	P-METHYLPHENOL
2348	CYCLOHEXANE	132		-0.10		C7H8O1	P-METHYLPHENOL
2349	CYCLOHEXANE	325		-0.19		C7H8O1	P-METHYLPHENOL
2350	OILS	327		1.21	2.28 A	C7H8O1	P-METHYLPHENOL
2351	N-BUTYL ACETATE	331		2.28	2.10	C7H8O1	P-METHYLPHENOL
2352	N-HEPTANE	310		-0.35		C7H8O1	P-METHYLPHENOL
2353	OLEYL ALCOHOL	124		1.80	2.35	C7H8O1	P-METHYLPHENOL
2354	PARAFFINS	327		-0.58		C7H8O1	P-METHYLPHENOL
2355	DIETHYL ETHER	332		1.23	1.20 A	C7H8O2	BENZENE,1,2-DIHYDROXY,4-METHYL
2356	DI-BUTYL ETHER	332		0.50		C7H8O2	BENZENE,1,2-DIHYDROXY,4-METHYL
2357	DI-I-PR. ETHER	332		0.94	1.64	C7H8O2	BENZENE,1,2-DIHYDROXY,4-METHYL
2358	OCTANOL	10		0.49	0.49 =	C7H8O2	M-HYDROXYBENZYL ALCOHOL
2359	OCTANOL	10		0.25	0.25 =	C7H8O2	P-HYDROXYBENZYL ALCOHOL
2360	OCTANOL	276		0.73	0.73 =	C7H8O2	O-HYDROXYBENZYLALCOHOL
2361	OCTANOL	10		1.58	1.58 =	C7H8O2	M-METHOXYPHENOL
2362	OLEYL ALCOHOL	124		1.15	1.70	C7H8O2	M-METHOXYPHENOL
2363	DIETHYL ETHER	323		1.36	1.31 A	C7H8O2	O-METHOXYPHENOL/GUAIACOL/
2364	OILS	224	12	1.48	2.53 A	C7H8O2	O-METHOXYPHENOL/GUAIACOL/
2365	OILS	327		0.96	2.06 A	C7H8O2	O-METHOXYPHENOL/GUAIACOL/
2366	OLEYL ALCOHOL	124		1.15	1.70	C7H8O2	O-METHOXYPHENOL/GUAIACOL/
2367	PARAFFINS	327		0.30		C7H8O2	O-METHOXYPHENOL/GUAIACOL/
2368	OCTANOL	10		1.34	1.34 =	C7H8O2	P-METHOXYPHENOL
2369	DIETHYL ETHER	323		1.36	1.31 A	C7H8O2	P-METHOXYPHENOL
2370	CYCLOHEXANE	56		-1.08		C7H8O2	P-METHOXYPHENOL
2371	OLEYL ALCOHOL	124		1.00	1.56	C7H8O2	P-METHOXYPHENOL
2372	OCTANOL	186		0.47	0.47 =	C7H8O2S1	SULFONE, METHYLPHENYL
2373	OCTANOL	56		0.50	0.50 =	C7H8O2S1	SULFONE, METHYLPHENYL
2374	OCTANOL	349		2.33	2.33 =	C7H8O2S1	THIOPHENE,2-CARBOXYLIC ACID, ETHYL ESTER
2375	OCTANOL	349		1.52	1.52 =	C7H8O3	FUROIC ACID, ETHYL ESTER
2376	DIETHYL ETHER	113	50	1.72	1.62 A	C7H8O3S1	BENZENESULFONIC ACID, METHYL ESTER
2377	CHCL3	113		2.98	3.39 N	C7H8O3S1	BENZENESULFONIC ACID, METHYL ESTER
2378	OCTANOL	56		2.74	2.74 =	C7H8S1	METHYLTHIOBENZENE
2379	BENZENE	311	6	-0.20		C7H9B1O2	M-METHYLPHENYLBORONIC ACID
2380	BENZENE	311	6	-0.16		C7H9B1O2	O-METHYLPHENYLBORONIC ACID
2381	BENZENE	311	6	-0.19		C7H9B1O2	P-METHYLPHENYLBORONIC ACID
2382	BENZENE	311	6	0.17		C7H9B1O2S1	P-METHYLTHIOPHENYLBORONIC ACID
2383	BENZENE	311	6	-0.43		C7H9B1O3	P-METHOXYPHENYLBORONIC ACID
2384	OCTANOL	373		-2.02	-2.02 =	C7H9CL1N2O1	N1-METHYLNICOTINAMIDE CHLORIDE
2385	OCTANOL	312		1.82	1.82 =	C7H9N1	ANILINE,N-METHYL
2386	OCTANOL	218		1.66	1.66 =	C7H9N1	ANILINE,N-METHYL
2387	CYCLOHEXANE	337		1.23		C7H9N1	ANILINE,N-METHYL
2388	OCTANOL	255		1.09	1.09 =	C7H9N1	BENZYLAMINE
2389	DIETHYL ETHER	3		0.28	1.11 B	C7H9N1	BENZYLAMINE
2390	DIETHYL ETHER	46		0.32	1.14 B	C7H9N1	BENZYLAMINE
2391	DIETHYL ETHER	374		0.36	1.14 B	C7H9N1	BENZYLAMINE
2392	CHCL3	46		1.18	0.78 B	C7H9N1	BENZYLAMINE
2393	BENZENE	315		0.61	0.97 B	C7H9N1	BENZYLAMINE
2394	1-BUTANOL	4		0.98	0.87	C7H9N1	BENZYLAMINE
2395	XYLENE	46		0.30	0.86 B	C7H9N1	BENZYLAMINE
2396	N-HEPTANE	315		-0.21		C7H9N1	BENZYLAMINE
2397	CHCL3	280		2.30		C7H9N1	2,6-LUTIDINE
2398	OCTANOL	10		1.40	1.40 =	C7H9N1	M-TOLUIDINE
2399	OCTANOL	301		1.43	1.43 =	C7H9N1	M-TOLUIDINE
2400	CYCLOHEXANE	337		0.64		C7H9N1	M-TOLUIDINE

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2401	CYCLOHEXANE	314		0.58		C7H9N1	M-TOLUIOINE
2402	BENZENE	314		1.50	1.59 B	C7H9N1	M-TOLUIOINE
2403	BENZENE	313		1.51	1.60 B	C7H9N1	M-TOLUIOINE
2404	BENZENE	72		1.28	1.43 B	C7H9N1	M-TOLUIOINE
2405	CCL4	314		1.15		C7H9N1	M-TOLUIOINE
2406	N-HEPTANE	310		0.54		C7H9N1	M-TOLUIOINE
2407	N-HEPTANE	314		0.45		C7H9N1	M-TOLUIOINE
2408	OCTANE	314		0.35		C7H9N1	M-TOLUIOINE
2409	OCTANOL	312		1.29	1.29 =	C7H9N1	O-TOLUIOINE
2410	OCTANOL	301		1.32	1.32 =	C7H9N1	O-TOLUIOINE
2411	CYCLOHEXANE	337		0.67		C7H9N1	O-TOLUIOINE
2412	CYCLOHEXANE	314		0.61		C7H9N1	O-TOLUIOINE
2413	BENZENE	314		1.53	1.61 B	C7H9N1	O-TOLUIOINE
2414	BENZENE	72		1.13	1.31 B	C7H9N1	O-TOLUIOINE
2415	CCL4	314		1.18		C7H9N1	O-TOLUIOINE
2416	N-HEPTANE	310		0.55		C7H9N1	O-TOLUIOINE
2417	N-HEPTANE	314		0.47		C7H9N1	O-TOLUIOINE
2418	OCTANE	314		0.37		C7H9N1	O-TOLUIOINE
2419	HEXAOECANE	314		0.38		C7H9N1	O-TOLUIOINE
2420	OCTANOL	10		1.39	1.39 =	C7H9N1	P-TOLUIDINE
2421	OCTANOL	301		1.41	1.41 =	C7H9N1	P-TOLUIOINE
2422	CYCLOHEXANE	337		0.58		C7H9N1	P-TOLUIOINE
2423	CYCLOHEXANE	314		0.55		C7H9N1	P-TOLUIOINE
2424	CHCL3	254		1.99	1.43 B	C7H9N1	P-TOLUIOINE
2425	BENZENE	314		1.43	1.54 B	C7H9N1	P-TOLUIOINE
2426	BENZENE	313		1.49	1.58 B	C7H9N1	P-TOLUIOINE
2427	BENZENE	72		1.38	1.52 B	C7H9N1	P-TOLUIOINE
2428	BENZENE	375		1.70	1.73 B	C7H9N1	P-TOLUIOINE
2429	CCL4	329		1.14	1.07 B	C7H9N1	P-TOLUIOINE
2430	CCL4	314		1.11		C7H9N1	P-TOLUIOINE
2431	N-HEPTANE	310		0.48		C7H9N1	P-TOLUIOINE
2432	N-HEPTANE	254		0.51		C7H9N1	P-TOLUIOINE
2433	N-HEPTANE	314		0.44		C7H9N1	P-TOLUIOINE
2434	HEXANE	314		0.41		C7H9N1	P-TOLUIOINE
2435	HEXANE	375		0.54		C7H9N1	P-TOLUIOINE
2436	OCTANE	314		0.33		C7H9N1	P-TOLUIOINE
2437	PARAFFINS	316		0.30		C7H9N1	P-TOLUIOINE
2438	HEXAOECANE	314		0.36		C7H9N1	P-TOLUIOINE
2439	OECANE	314		0.37		C7H9N1	P-TOLUIOINE
2440	OCTANOL	10		-0.05	-0.05 =	C7H9N1O1	M-AMINOBENZYL ALCOHOL
2441	OCTANOL	312		0.93	0.93 =	C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2442	OCTANOL	10		0.93	0.93 =	C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2443	CYCLOHEXANE	314		-0.13		C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2444	BENZENE	314		1.12	1.32 B	C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2445	CCL4	314		0.63		C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2446	N-HEPTANE	314		-0.28		C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2447	HEXAOECANE	314		-0.33		C7H9N1O1	M-METHOXYANILINE/M-ANISIOINE/
2448	OCTANOL	312		0.95	0.95 =	C7H9N1O1	O-METHOXYANILINE/O-ANISIOINE/
2449	CYCLOHEXANE	314		0.52		C7H9N1O1	O-METHOXYANILINE/O-ANISIOINE/
2450	BENZENE	314		1.59	1.65 B	C7H9N1O1	O-METHOXYANILINE/O-ANISIOINE/
2451	CCL4	314		1.22		C7H9N1O1	O-METHOXYANILINE/O-ANISIOINE/
2452	N-HEPTANE	314		0.39		C7H9N1O1	O-METHOXYANILINE/O-ANISIOINE/
2453	HEXAOECANE	314		0.33		C7H9N1O1	O-METHOXYANILINE/O-ANISIOINE/
2454	OCTANOL	312		0.95	0.95 =	C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2455	CYCLOHEXANE	314		-0.41		C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2456	BENZENE	314		0.87	1.15 B	C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2457	BENZENE	72		0.78	1.09 B	C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2458	CCL4	314		0.38		C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2459	N-HEPTANE	314		-0.54		C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2460	HEXAOECANE	314		-0.54		C7H9N1O1	P-METHOXYANILINE/P-ANISIOINE/
2461	OIETHYL ETHER	113		0.80	0.81 A	C7H9N1O2S1	BENZENESULFONAMIOE,N-METHYL
2462	CHCL3	113		1.31	1.84 N	C7H9N1O2S1	BENZENESULFONAMIOE,N-METHYL
2463	OCTANOL	217	07	0.85	0.85 =	C7H9N1O2S1	M-METHYLBENZENESULFONAMIOE
2464	CHCL3	217	07	0.32	0.85 N	C7H9N1O2S1	M-METHYLBENZENESULFONAMIOE
2465	OCTANOL	217	07	0.84	0.84 =	C7H9N1O2S1	O-METHYLBENZENESULFONAMIOE
2466	CHCL3	217	07	0.46	0.96 N	C7H9N1O2S1	O-METHYLBENZENESULFONAMIOE
2467	OCTANOL	217	07	0.82	0.82 =	C7H9N1O2S1	P-METHYLBENZENESULFONAMIOE
2468	CHCL3	217	07	0.33	0.86 N	C7H9N1O2S1	P-METHYLBENZENESULFONAMIOE
2469	OCTANOL	217	07	0.47	0.47 =	C7H9N1O3S1	P-METHOXYBENZENESULFONAMIOE
2470	CHCL3	217	07	0.15	0.70 N	C7H9N1O3S1	P-METHOXYBENZENESULFONAMIOE
2471	OIETHYL ETHER	113		0.37	0.44 A	C7H9N3O2S2	SULFATHIOCARBAMIOE
2472	CHCL3	113		-0.78	-0.12 N	C7H9N3O2S2	SULFATHIOCARBAMIOE
2473	OIETHYL ETHER	113		-1.25	-0.98 A	C7H9N3O3S1	SULFACARBAMIOE
2474	CHCL3	113	15	-2.16	-1.41 N	C7H9N3O3S1	SULFACARBAMIOE
2475	CHCL3	322		-0.14	-0.24 B	C7H9N5	6-OIMETHYLAMINOPURINE
2476	BENZENE	311	6	-1.83		C7H10B1N1O2	PHENYLBORONIC ACIO,3-AMINO,4-METHYL
2477	OCTANOL	341	60	0.39	0.39 =	C7H10N2	N-METHYL-3-PYRIOYLMETHYLAMINE
2478	OCTANOL	341	60	-0.11	-0.11 =	C7H10N2	3-PYRIOYLETHYLAMINE
2479	OCTANOL	217	32	0.08	0.08 =	C7H10N2O2S1	P-METHYLAMINOBENZENESULFONAMIOE
2480	CHCL3	217	32	-0.59	0.03 N	C7H10N2O2S1	P-METHYLAMINOBENZENESULFONAMIOE
2481	OCTANOL	56		-1.22	-1.22 =	C7H10N4O2S1	SULFAGUANIDINE
2482	OIETHYL ETHER	113		-2.61	-1.47 B	C7H10N4O2S1	SULFAGUANIDINE
2483	CHCL3	343	2	-2.00	-1.26 N	C7H10N4O2S1	SULFAGUANIOINE
2484	CHCL3	113	12	-3.20	-2.38 N	C7H10N4O2S1	SULFAGUANIOINE
2485	BENZENE	343	2	-1.47	-0.47 B	C7H10N4O2S1	SULFAGUANIDINE
2486	1-PENT. ACETATE	343	2	-1.52	-1.75	C7H10N4O2S1	SULFAGUANIDINE
2487	CCL4	343	2	-3.00	-3.37 N	C7H10N4O2S1	SULFAGUANIDINE
2488	N-BUTANOL	194		0.07	-0.46	C7H10O6	B-CARBOXYAOIPIC ACIO
2489	ETHYL ACETATE	194		-0.50	-0.62	C7H10O6	B-CARBOXYAOIPIC ACIO
2490	CYCLOHEXANONE	194		0.13		C7H10O6	B-CARBOXYAOIPIC ACIO
2491	2-BUTANONE	194		0.00	-0.68	C7H10O6	B-CARBOXYAOIPIC ACID
2492	ME-1-BUT.KETONE	194		-0.83	-2.35	C7H10O6	B-CARBOXYAOIPIC ACIO
2493	OCTANOL	348		-0.40	-0.40 =	C7H11N1O2	N-ACETYLCYCLOBUTANECARBOXAMIOE
2494	CHCL3	67		-1.18		C7H11N1O3	ACETYLPROLINE
2495	HEXANE	376		-0.59		C7H11N1O3	N-METHYLCARBAMIC ACIO,2,3-DIHYORO-2-MEFURANYL ESTER
2496	ETHYL ACETATE	67		-1.36	-1.52	C7H11N1O5	GLUTAMIC ACIO,L,N-ACETYL
2497	CHCL3	265		-0.70	-0.05 N	C7H12N2O2	CYCLOHEPTANEOIONE OIOXIME
2498	OCTANOL	134		1.01	1.01 =	C7H12N4O1S1	3-METHIO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
2499	OCTANOL	134		0.93	0.93 =	C7H12N4O1S1	3-METHIO-4-AMINO-6-N-PR-1,2,4-TRIAZINE-5-ONE
2500	OCTANOL	134		-0.06	-0.06 =	C7H12N4O2	3-METHOXY-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2501	OCTANOL	255		1.50	1.50 =	C7H12O1	2-BUTANONE,4-CYCLOPROPYL
2502	DIETHYL ETHER	3		1.04	1.03 A	C7H12O4	DIETHYLMALONIC ACID
2503	I-BUTANOL	4		1.22	1.21	C7H12O4	DIETHYLMALONIC ACID
2504	DIETHYL ETHER	212		0.17	0.26 A	C7H12O4	PIMELIC ACID
2505	DIETHYL ETHER	212		0.18	0.27 A	C7H12O4	PIMELIC ACID
2506	DIETHYL ETHER	207		0.14	0.24 A	C7H12O4	PIMELIC ACID
2507	DIETHYL ETHER	194		0.04	0.14 A	C7H12O4	PIMELIC ACID
2508	N-BUTANOL	194		0.77	0.58	C7H12O4	PIMELIC ACID
2509	I-BUTANOL	4		0.86	0.70	C7H12O4	PIMELIC ACID
2510	ETHYL ACETATE	194		0.43	0.41	C7H12O4	PIMELIC ACID
2511	DIETHYL ETHER	3		-0.66	-0.46 A	C7H12O5	GLYCERYL DIACETATE
2512	OILS	2		-1.15	-0.51 B	C7H12O5	GLYCERYL DIACETATE
2513	OILS	2		-1.15	0.14 A	C7H12O5	GLYCERYL DIACETATE
2514	OILS	214	12	-0.64	0.65 A	C7H12O5	GLYCERYL DIACETATE
2515	DIETHYL ETHER	3		-3.51	-1.90 B	C7H12O6	CYCLOHEXANECARBOXYLIC ACID,1,3,4,5-TETRAHYDROXY/QUINIC/
2516	I-BUTANOL	4		-1.09	-2.04	C7H12O6	CYCLOHEXANECARBOXYLIC ACID,1,3,4,5-TETRAHYDROXY/QUINIC/
2517	OILS	296		0.52	1.66 A	C7H13BR1N2O2	A-BROMO-A-ETHYLBUTYRLUREA/CARBROMAL/
2518	OLEYL ALCOHOL	82		0.81	1.37	C7H13BR1N2O2	A-BROMO-A-ETHYLBUTYRLUREA/CARBROMAL/
2519	OCTANOL	260		0.24	0.24 =	C7H13N1O1	2-AZACYCLOOCTANONE
2520	CHCL3	67		-1.48		C7H13N1O3	L-VALINE,ACETYL
2521	CHCL3	67		-1.34		C7H13N1O3S1	L-METHIONINE,ACETYL
2522	OCTANOL	260		1.00	1.00 =	C7H13N1S1	2-AZACYCLOOCTANTHIONE
2523	OCTANOL	134		0.30	0.30 =	C7H13N5O1	6-I-PROPYL-4-AMINO-3-MEAMINO-1,2,4-TRIAZIN-5-ONE
2524	DIETHYL ETHER	3		-1.92	-0.82 B	C7H14N2O2	DIETHYLMALONIC ACID DIAMIDE
2525	PARAFFINS	241		-1.02		C7H14N2S1	N-BUTYLETHYLENETHIOUREA
2526	XYLENE	46		1.24	3.13 A	C7H14O2	I-AMYLACETIC ACID
2527	OILS	220		1.69	2.72 A	C7H14O2	HEPTANOIC ACID
2528	OCTANE	60	47	-0.13		C7H14O2	HEPTANOIC ACID
2529	DODECANE	60	47	-0.18		C7H14O2	HEPTANOIC ACID
2530	HEXADECANE	60	47	-0.29		C7H14O2	HEPTANOIC ACID
2531	OCTANOL	268		-0.17	-0.17 =	C7H14O4	GLYCERYLMONOBUTYRATE/BUTYRIN/
2532	I-BUTANOL	4		-1.41	-2.48	C7H14O6	A-METHYLGLUCOSIDE
2533	OCTANOL	227		0.63	0.63 =	C7H15CL2N2O2P1	CYTOXAN/CYCLOPHOSPHAMIDE/
2534	CCL4	234	12	0.32		C7H15N1O1	DIETHYLPROPIONAMIDE
2535	OILS	292		-0.38	0.84 A	C7H15N1O1	N,N-DIMETHYLVALERAMIDE
2536	OILS	292		-0.59	0.65 A	C7H15N1O1	N-ETHYLVALERAMIDE
2537	OILS	292		-0.81	0.45 A	C7H15N1O2	N,N-DIETHYLLACTAMIDE
2538	N-BUTANOL	377		-0.77	-1.59	C7H16CL1N1O2	ACETYLCHOLINE CHLORIDE
2539	OCTANOL	297	46	-0.25	-0.25 =	C7H16N1O2	ACETYLCHOLINE CATION
2540	DIETHYL ETHER	378	44	-1.03	0.04 B	C7H16N2O2	CARBAMIC ACID,N,N-DIETHYLAMINOETHYL ESTER
2541	OILS	201		1.34	2.41 A	C7H16O1	HEPTANOL
2542	OCTANE	59		0.93		C7H16O1	HEPTANOL
2543	DODECANE	59		0.86		C7H16O1	HEPTANOL
2544	HEXADECANE	59		0.77		C7H16O1	HEPTANOL
2545	DIETHYL ETHER	3		-0.07	0.05 A	C7H16O3	GLYCEROL,1,3-DIETHYL ETHER
2546	OILS	2		-0.96	0.37 A	C7H16O3	GLYCEROL,1,3-DIETHYL ETHER
2547	OILS	214		0.05	0.48 B	C7H16O4S2	2,2-BIS(ETHYLSULFONYL) PROPANE /SULFONAL/
2548	OILS	173		0.18	0.58 B	C7H16O4S2	2,2-BIS(ETHYLSULFONYL)PROPANE/SULFONAL/
2549	OILS	224		0.65	0.98 B	C7H16O4S2	2,2-BIS(ETHYLSULFONYL)PROPANE/SULFONAL/
2550	OILS	168		0.10	0.52 B	C7H16O4S2	2,2-BIS(ETHYLSULFONYL(PROPANE/SULFONAL/
2551	DIETHYL ETHER	46		1.30	2.02 B	C7H17N1	HEPTYLAMINE
2552	XYLENE	46		1.34	2.09 B	C7H17N1	HEPTYLAMINE
2553	OCTANOL	297	46	-2.60	-2.60 =	C7H18I1N1	TRIMETHYLBUTYLAMMONIUM IODIDE
2554	OCTANOL	298		4.20	4.20 =	C7H18SI1	SILANE, BUTYL-TRIMETHYL
2555	OCTANOL	206		4.81	4.81 =	C8H1BR4F3N2	BENZIMIDAZOLE,4,5,6,7-TETRABROMO-2-TRIFLUOROMETHYL
2556	CYCLOHEXANE	379	19	-0.26		C8H1CL2F3N4O4	BENZIMIDAZOLE,2-TRIFLME-4,6-DICL-5,7-DINITRO
2557	CYCLOHEXANE	379	19	0.94		C8H1CL4F3N2	BENZIMIDAZOLE,4,5,6,7TETRACHLORO-2-TRIFLUOROME
2558	OCTANOL	206		3.97	3.97 =	C8H1CL4F3N2	BENZIMIDAZOLE,4,5,6,7-TETRACHLORO-2-TRIFLUOROMETHYL
2559	OCTANOL	206		4.08	4.08 =	C8H2BR3F3N2	BENZIMIDAZOLE,4,5,6-TRIBROMO-2-TRIFLUOROMETHYL
2560	OCTANOL	206		3.78	3.78 =	C8H2CL3F3N2	BENZIMIDAZOLE,4,5,7-TRICHLORO-2-TRIFLUOROMETHYL
2561	OCTANOL	206		3.87	3.87 =	C8H2CL3F3N2	BENZIMIDAZOLE,4,5,6-TRICHLORO-2-TRIFLUOROMETHYL
2562	CYCLOHEXANE	379	19	0.57		C8H2CL3F3N2	BENZIMIDAZOLE,4,5,6-TRICHLORO-2-TRIFLUOROMETHYL
2563	CYCLOHEXANE	379	19	0.42		C8H2CL3F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-4,6,7-TRICHLORO
2564	OCTANOL	206		4.15	4.15 =	C8H3BR2F3N2	BENZIMIDAZOLE,2-TRIFLUOROMETHYL-5,6-DIBROMO
2565	OCTANOL	206		3.21	3.21 =	C8H3CL1F3N3O2	BENZIMIDAZOLE,5-CHLORO-6-NITRO-2-TRIFLUOROME
2566	CYCLOHEXANE	379	19	-0.74		C8H3CL1F3N3O2	BENZIMIDAZOLE,2-TRIFLME-4,CHLORO-6-NITRO
2567	CYCLOHEXANE	379	19	-0.06		C8H3CL1F3N3O2	BENZIMIDAZOLE,2-TRIFLME-6-CHLORO-5-NITRO
2568	CYCLOHEXANE	379	19	0.37		C8H3CL1F3N3O2	BENZIMIDAZOLE,2-TRIFLME-6-CHLORO-4-NITRO
2569	OCTANOL	206		2.87	2.87 =	C8H3CL2F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-4,7-DICHLORO
2570	OCTANOL	206		3.49	3.49 =	C8H3CL2F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-4,5-DICHLORO
2571	OCTANOL	206		3.49	3.49 =	C8H3CL2F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-4,6-DICHLORO
2572	OCTANOL	206		3.99	3.99 =	C8H3CL2F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-5,6-DICHLORO
2573	CYCLOHEXANE	379	19	0.30		C8H3CL2F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-4,5-DICHLORO
2574	OCTANOL	206		3.89	3.89 =	C8H3F3N4O4	BENZIMIDAZOLE,2-TRIFLUOROME-5,6-DINITRO
2575	CYCLOHEXANE	379	19	-1.10		C8H3F3N4O4	BENZIMIDAZOLE,2-TRIFLUOROME-5,6-DINITRO
2576	CYCLOHEXANE	379	19	-0.82		C8H3F3N4O4	BENZIMIDAZOLE,2-TRIFLUOROME-4,6-DINITRO
2577	OCTANOL	206		3.57	3.57 =	C8H4BR1F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-5-BROMO
2578	OCTANOL	206		3.39	3.39 =	C8H4CL1F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-5-CHLORO
2579	CYCLOHEXANE	379	19	-0.31		C8H4CL1F3N2	BENZIMIDAZOLE,2-TRIFLUOROME-5-CHLORO
2580	OCTANOL	206		2.93	2.93 =	C8H4CL1F3N2	BENZIMIDAZOLE,2-TRIFLUROME-4-CHLORO
2581	OCTANOL	235		4.62	4.62 =	C8H4CL6	P-DI(TRICHLOROMETHYL)BENZENE
2582	OCTANOL	206		2.68	2.68 =	C8H4F3N3O2	BENZIMIDAZOLE,2-TRIFLUOROME-5-NITRO
2583	CYCLOHEXANE	379	19	-1.70		C8H4F3N3O2	BENZIMIDAZOLE,2-TRIFLUOROME-5-NITRO
2584	CYCLOHEXANE	379	19	-0.10		C8H4F3N3O2	BENZIMIDAZOLE,2-TRIFLUOROME-4-NITRO
2585	OCTANOL	218		3.34	3.34 =	C8H5BR1F3N1O1	BROMOBENZENE,P-TRIFLUOROACETAMIDO
2586	CYCLOHEXANE	141		1.66		C8H5BR1N2O4	STYRENE,2-BROMO,5-NITRO,B-NITRO
2587	OCTANOL	141		2.23	2.23 =	C8H5CL1N2O4	STYRENE, 2-CHLORO-5-NITRO-B-NITRO
2588	CYCLOHEXANE	141		1.49		C8H5CL1N2O4	STYRENE,2-CHLORO,5-NITRO,B-NITRO
2589	OCTANOL	141		2.53		C8H5CL2N1O2	STYRENE,2,4-DICHLORO-B-NITRO
2590	CYCLOHEXANE	141		2.68		C8H5CL2N1O2	STYRENE,3,4-DICHLORO,B-NITRO
2591	CYCLOHEXANE	141		2.76		C8H5CL2N1O2	STYRENE,2,4-DICHLORO,B-NITRO
2592	CYCLOHEXANE	141		3.12		C8H5CL2N1O2	STYRENE,2,6-DICHLORO,B-NITRO
2593	CYCLOHEXANE	141		0.31		C8H5F1N2O4	STYRENE,4-FLUORO,3-NITRO,B-NITRO
2594	CYCLOHEXANE	141		0.87		C8H5F1N2O4	STYRENE,2-FLUORO,5-NITRO,B-NITRO
2595	OCTANOL	206		2.67	2.67 =	C8H5F3N2	BENZIMIDAZOLE,2-TRIFLUOROMETHYL
2596	CYCLOHEXANE	379	19	-0.95		C8H5F3N2	BENZIMIDAZOLE,2-TRIFLUOROMETHYL
2597	OCTANOL	10		2.95	2.95 =	C8H5F3O2	M-TRIFLUOROMETHYLBENZOIC ACID
2598	CHCL3	279		1.73	2.79 A	C8H5F3O2S1	THENOYL-TRIFLUOROACETONE
2599	BENZENE	380		1.60	2.95 A	C8H5F3O2S1	THENOYL-TRIFLUOROACETONE
2600	BENZENE	279		1.62	2.96 A	C8H5F3O2S1	THENOYL-TRIFLUOROACETONE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2601	CCL4	279		1.30	2.54 N	C8H5F3O2S1	THENOYLTRIFLUOROACETONE
2602	HEXANE	279		0.68		C8H5F3O2S1	THENOYLTRIFLUOROACETONE
2603	O-DICL. BENZENE	279		1.59		C8H5F3O2S1	THENOYLTRIFLUOROACETONE
2604	XYLENE	279		1.58		C8H5F3O2S1	THEONYLTRIFLUOROACETONE
2605	TOLUENE	279		1.60	2.98 A	C8H5F3O2S1	THEONYLTRIFLUOROACETONE
2606	OCTANOL	10		1.48	1.48 =	C8H5N1O2	M-CYANOBENZOIC ACID
2607	OCTANOL	10		1.56	1.56 =	C8H5N1O2	P-CYANOBENZOIC ACID
2608	DIETHYL ETHER	113		0.31	1.12 B	C8H5N1O2	INDOLE,2,3-DIONE/ISATIN/
2609	CHCL3	113		0.23	0.80 N	C8H5N1O2	INDOLE,2,3-DIONE/ISATIN/
2610	OCTANOL	9		1.15	1.15 =	C8H5N1O2	PHTHALIMIDE
2611	DIETHYL ETHER	113		1.03	1.02 A	C8H5N1O2	PHTHALIMIDE
2612	CYCLOHEXANE	304		-1.46		C8H5N1O2	PHTHALIMIDE
2613	CHCL3	113		1.08	1.60 N	C8H5N1O2	PHTHALIMIDE
2614	OILS	381	12	0.55	1.69 A	C8H5N1O2	PHTHALIMIDE
2615	OCTANOL	255		2.53	2.53 =	C8H6	BENZENE,ETHYNYL
2616	OCTANOL	302		2.75	2.75 =	C8H6BR1CL1O3	PHENOXYACETIC ACID,3-BROMO-4-CHLORO
2617	OCTANOL	309		3.00	3.00 =	C8H6BR1N1	INDOLE, 5-BROMO
2618	CYCLOHEXANE	141		2.33		C8H6BR1N1O2	STYRENE,4-BROMO,B-NITRO
2619	CYCLOHEXANE	141		2.44		C8H6BR1N1O2	STYRENE,2-BROMO,B-NITRO
2620	CYCLOHEXANE	141		2.48		C8H6BR1N1O2	STYRENE,3-BROMO,B-NITRO
2621	OCTANOL	302		2.20	2.20 =	C8H6CL1F1O3	PHENOXYACETIC ACID,3-CHLORO-5-FLUORO
2622	OCTANOL	302		3.10	3.10 =	C8H6CL1I1O3	PHENOXYACETIC ACID,4-CHLORO-3-IODO
2623	OCTANOL	141		2.44	2.44 =	C8H6CL1N1O2	STYRENE, 4-CHLORO-B-NITRO
2624	OCTANOL	141		2.57	2.57 =	C8H6CL1N1O2	STYRENE, 3-CHLORO-B-NITRO
2625	OCTANOL	141		2.85	2.85 =	C8H6CL1N1O2	STYRENE, 2-CHLORO-B-NITRO
2626	CYCLOHEXANE	141		2.24		C8H6CL1N1O2	STYRENE,4-CHLORO,B-NITRO
2627	CYCLOHEXANE	141		2.33		C8H6CL1N1O2	STYRENE,3-CHLORO,B-NITRO
2628	CYCLOHEXANE	141		2.52		C8H6CL1N1O2	STYRENE,2-CHLORO,B-NITRO
2629	OCTANOL	302		1.85	1.85 =	C8H6CL1N1O5	PHENOXYACETIC ACID,4-CHLORO-3-NITRO
2630	OCTANOL	10		2.81	2.81 =	C8H6CL2O3	PHENOXYACETIC ACID,2,4-DICHLORO
2631	OCTANOL	218		2.81	2.81 =	C8H6CL2O3	PHENOXYACETIC ACID,3,4-DICHLORO
2632	OCTANOL	302		2.42	2.42 =	C8H6F1I1O3	PHENOXYACETIC ACID,5-FLUORO-3-IODO
2633	CYCLOHEXANE	141		1.61		C8H6F1N1O2	STYRENE,4-FLUORO,B-NITRO,
2634	CYCLOHEXANE	141		1.74		C8H6F1N1O2	STYRENE,3-FLUORO,B-NITRO
2635	CYCLOHEXANE	141		1.94		C8H6F1N1O2	STYRENE,2-FLUORO,B-NITRO
2636	OILS	382	24	3.55	4.42 A	C8H6I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,METHYL ESTER
2637	OCTANOL	360		0.84	0.84 =	C8H6N2	QUINOXALINE
2638	OCTANOL	141		1.80	1.80 =	C8H6N2O4	STYRENE,2-NITRO-B-NITRO
2639	OCTANOL	141		1.82	1.82 =	C8H6N2O4	STYRENE,3-NITRO-B-NITRO
2640	OCTANOL	141		1.89	1.89 =	C8H6N2O4	STYRENE,4-NITRO-B-NITRO
2641	CYCLOHEXANE	141		0.72		C8H6N2O4	STYRENE,4-NITRO,B-NITRO
2642	CYCLOHEXANE	141		0.89		C8H6N2O4	STYRENE,2-NITRO,B-NITRO
2643	CYCLOHEXANE	141		1.01		C8H6N2O4	STYRENE,3-NITRO,B-NITRO
2644	OCTANOL	276		1.63	1.63 =	C8H6N4O4	1-METHYL-5,7-DINITROBENZPYRAZOLE
2645	OCTANOL	218		2.67	2.67 =	C8H6O1	BENZOFURAN
2646	OILS	224		0.52	0.88 B	C8H6O2	O-TOLUIC ACID LACTONE/PHTHALIDE/
2647	DIETHYL ETHER	207		0.80	0.82 A	C8H6O3	BENZOYLFORMIC ACID
2648	OILS	173		1.47	1.61 B	C8H6O3	PIPERONAL
2649	OILS	224	12	2.00		C8H6O3	PIPERONAL
2650	OCTANOL	10		1.66	1.66 =	C8H6O4	M-PHTHALIC ACID
2651	DIETHYL ETHER	212		1.46	1.39 A	C8H6O4	M-PHTHALIC ACID
2652	DIETHYL ETHER	212		0.20	0.29 A	C8H6O4	O-PHTHALIC ACID
2653	DIETHYL ETHER	207		0.10	0.20 A	C8H6O4	O-PHTHALIC ACID
2654	DIETHYL ETHER	46		0.28	0.37 A	C8H6O4	O-PHTHALIC ACID
2655	1-BUTANOL	4		0.86	0.70	C8H6O4	O-PHTHALIC ACID
2656	XYLENE	46		-1.55	0.10 A	C8H6O4	O-PHTHALIC ACID
2657	ME-I-BUT.KETONE	195		0.44	0.41	C8H6O4	O-PHTHALIC ACID
2658	S-PENTANOLS	195		0.60	0.38	C8H6O4	O-PHTHALIC ACID
2659	CHCL3	46		0.70	1.85 A	C8H6O4	PIPERONYLIC ACID
2660	OCTANOL	218		3.12	3.12 =	C8H6S1	BENZOTHIOPHENE,(B)
2661	OCTANOL	309		3.09	3.09 =	C8H6S1	BENZOTHIOPHENE,(B)
2662	OILS	173		2.24	2.29 B	C8H7BR1O1	BROMOACETOPHENONE
2663	OCTANOL	10		2.37	2.37 =	C8H7BR1O2	M-BROMOPHENYLACETIC ACID
2664	OCTANOL	10		2.31	2.31 =	C8H7BR1O2	P-BROMOPHENYLACETIC ACID
2665	OILS	383	12	1.86	2.88 A	C8H7BR1O2	P-BROMOPHENYLACETIC ACID
2666	OCTANOL	10		2.10	2.10 =	C8H7BR1O3	PHENOXYACETIC ACID,2-BROMO
2667	OCTANOL	10		2.22	2.22 =	C8H7BR1O3	PHENOXYACETIC ACID,3-BROMO
2668	OCTANOL	10		2.45	2.45 =	C8H7BR1O3	PHENOXYACETIC ACID,4-BROMO
2669	OCTANOL	206		3.22	3.22 =	C8H7CL1N2S1	BENZIMIDAZOLE,5-CHLORO-2-(METHYLTHIO)
2670	CYCLOHEXANE	304		1.44		C8H7CL1O1	CHLOROACETEPHENONE
2671	OILS	173		1.99	2.08 B	C8H7CL1O1	CHLOROACETOPHENONE
2672	OCTANOL	10		2.09	2.09 =	C8H7CL1O2	M-CHLOROPHENYLACETIC ACID
2673	OCTANOL	10		2.12	2.12 =	C8H7CL1O2	P-CHLOROPHENYLACETIC ACID
2674	OILS	383		1.38	2.48 A	C8H7CL1O2	P-CHLOROPHENYLACETIC ACID
2675	OCTANOL	10		2.03	2.03 =	C8H7CL1O3	PHENOXYACETIC ACID,M-CHLORO
2676	CYCLOHEXANONE	302		3.00		C8H7CL1O3	PHENOXYACETIC ACID,M-CHLORO
2677	ME-I-BUT.KETONE	302		2.32		C8H7CL1O3	PHENOXYACETIC ACID,M-CHLORO
2678	CYCLOHEXANOL	302		2.46		C8H7CL1O3	PHENOXYACETIC ACID,M-CHLORO
2679	OCTANOL	10		2.02	2.02 =	C8H7CL1O3	PHENOXYACETIC ACID,O-CHLORO
2680	OCTANOL	10		1.99	1.99 =	C8H7CL1O3	PHENOXYACETIC ACID,P-CHLORO
2681	OCTANOL	384		2.80	2.80 =	C8H7CL2N1O2	N-METHYL-3,4-DICHLOROPHENYLCARBAMATE
2682	OCTANOL	384		3.03	3.03 =	C8H7CL2N1O2	N-METHYL-3,5-DICHLOROPHENYLCARBAMATE
2683	OCTANOL	10		1.65	1.65 =	C8H7F1O2	M-FLUOROPHENYLACETIC ACID
2684	OCTANOL	10		1.50	1.50 =	C8H7F1O2	O-FLUOROPHENYLACETIC ACID
2685	OCTANOL	10		1.55	1.55 =	C8H7F1O2	P-FLUOROPHENYLACETIC ACID
2686	OCTANOL	10		1.48	1.48 =	C8H7F1O3	PHENOXYACETIC ACID,M-FLUORO
2687	OCTANOL	10		1.26	1.26 =	C8H7F1O3	PHENOXYACETIC ACID,O-FLUORO
2688	OCTANOL	10		1.41	1.41 =	C8H7F1O3	PHENOXYACETIC ACID,P-FLUORO
2689	CYCLOHEXANOL	302		1.82		C8H7F1O3	PHENOXYACETIC ACID,P-FLUORO
2690	OCTANOL	65		1.86	1.86 =	C8H7F1O4S1	P-FLUOROSULFONYLPHENYLACETIC ACID
2691	OCTANOL	65		1.82	1.82 =	C8H7F1O5S1	P-FLUOROSULFONYLPHENOXYACETIC ACID
2692	OCTANOL	10		2.78	2.78 =	C8H7F5O3S1	PHENOXYACETIC ACID,3-PENTAFLUOROTHIO
2693	OCTANOL	10		2.62	2.62 =	C8H7I1O2	M-IODOPHENYLACETIC ACID
2694	OCTANOL	10		2.64	2.64 =	C8H7I1O2	P-IODOPHENYLACETIC ACID
2695	OILS	383		1.63	2.72 A	C8H7I1O2	P-IODOPHENYLACETIC ACID
2696	OCTANOL	10		2.19	2.19 =	C8H7I1O3	PHENOXYACETIC ACID,2-IODO
2697	OCTANOL	10		2.44	2.44 =	C8H7I1O3	PHENOXYACETIC ACID,3-IODO
2698	OCTANOL	10		2.69	2.69 =	C8H7I1O3	PHENOXYACETIC ACID,4-IODO
2699	OCTANOL	276		2.00	2.00 =	C8H7N1	INDOLE
2700	OCTANOL	186		2.14	2.14 =	C8H7N1	INDOLE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2701	OCTANOL	309		2.25	2.25 =	C8H7N1	INDOLE
2702	OCTANOL	255		1.56	1.56 =	C8H7N1	PHENYLACETONITRILE
2703	CYCLOHEXANE	358		1.56		C8H7N1	P-TOLUONITRILE
2704	OCTANOL	309		1.15	1.15 =	C8H7N1O1	OXINDOLE
2705	OCTANOL	56		2.24	2.24 =	C8H7N1O2	STYRENE, B-NITRO
2706	OCTANOL	141		2.11	2.11 =	C8H7N1O2	STYRENE, B-NITRO
2707	CYCLOHEXANE	141		1.80		C8H7N1O2	STYRENE,B-NITRO
2708	OCTANOL	10		1.42	1.42 =	C8H7N1O3	M-ACETYLNITROBENZENE
2709	OCTANOL	10		1.49	1.49 =	C8H7N1O3	P-ACETYLNITROBENZENE
2710	OCTANOL	141		2.07	2.07 =	C8H7N1O3	STYRENE, 3-HYDROXY-B-NITRO
2711	OCTANOL	141		2.12	2.12 =	C8H7N1O3	STYRENE, 4-HYDROXY-B-NITRO
2712	CYCLOHEXANE	141		-1.60		C8H7N1O3	STYRENE,4-HYDROXY,B-NITRO
2713	CYCLOHEXANE	141		-1.36		C8H7N1O3	STYRENE,3-HYDROXY,B-NITRO
2714	OCTANOL	10		1.45	1.45 =	C8H7N1O4	M-NITROPHENYLACETIC ACID
2715	OCTANOL	10		1.39	1.39 =	C8H7N1O4	P-NITROPHENYLACETIC ACID
2716	OILS	383		0.43	1.61 A	C8H7N1O4	P-NITROPHENYLACETIC ACID
2717	OCTANOL	10		1.37	1.37 =	C8H7N1O5	PHENOXYACETIC ACID,M-NITRO
2718	CYCLOHEXANONE	302		2.77		C8H7N1O5	PHENOXYACETIC ACID,M-NITRO
2719	ME-1-BUT.KETONE	302		1.88		C8H7N1O5	PHENOXYACETIC ACID,M-NITRO
2720	CYCLOHEXANOL	302		1.93		C8H7N1O5	PHENOXYACETIC ACID,M-NITRO
2721	OCTANOL	10		1.22	1.22 =	C8H7N1O5	PHENOXYACETIC ACID,O-NITRO
2722	OCTANOL	10		1.48	1.48 =	C8H7N1O5	PHENOXYACETIC ACID,P-NITRO
2723	OCTANOL	238		2.83	2.83 =	C8H7N1S1	BENZYLISOTHIOCYANATE
2724	CHCL3	322		2.00	2.38 N	C8H7N1S2	METHYLTHIOBENZOTHIAZOLE
2725	OCTANOL	384		1.77	1.77 =	C8H8BR1N1O2	N-METHYL-2-BROMOPHENYLCARBAMATE
2726	OCTANOL	384		2.25	2.25 =	C8H8BR1N1O2	N-METHYL-3-BROMOPHENYLCARBAMATE
2727	OCTANOL	384		2.17	2.17 =	C8H8BR1N1O2	N-METHYL-4-BROMOPHENYLCARBAMATE
2728	OCTANOL	384		1.64	1.64 =	C8H8CL1N1O2	N-METHYL-2-CHLOROPHENYLCARBAMATE
2729	OCTANOL	384		2.03	2.03 =	C8H8CL1N1O2	N-METHYL-3-CHLOROPHENYLCARBAMATE
2730	OCTANOL	384		2.01	2.01 =	C8H8CL1N1O2	N-METHYL-4-CHLOROPHENYLCARBAMATE
2731	OCTANOL	302		1.16	1.16 =	C8H8CL1N1O3	PHENOXYACETIC ACID,3-AMINO-4-CHLORO
2732	OCTANOL	384		1.25	1.25 =	C8H8F1N1O2	N-METHYL-2-FLUOROPHENYLCARBAMATE
2733	OCTANOL	384		1.48	1.48 =	C8H8F1N1O2	N-METHYL-3-FLUOROPHENYLCARBAMATE
2734	OCTANOL	384		1.28	1.28 =	C8H8F1N1O2	N-METHYL-4-FLUOROPHENYLCARBAMATE
2735	OCTANOL	65		2.17	2.17 =	C8H8F1N1O3S1	P-ACETAMIDO-BENZENESULFONYLFLUORIDE
2736	DIETHYL ETHER	306		1.64	1.60 A	C8H8I1N1O4S1	N-(P-IODOBENZENESULFONYL)GLYCINE
2737	CHCL3	306		-0.20	1.00 A	C8H8I1N1O4S1	N-(P-IODOBENZENESULFONYL)GLYCINE
2738	CCL4	306	12	-2.00	0.15 A	C8H8I1N1O4S1	N-(P-IODOBENZENESULFONYL)GLYCINE
2739	CLCH2CH2CL	306		0.32		C8H8I1N1O4S1	N-(P-IODOBENZENESULFONYL)GLYCINE
2740	OCTANOL	384		1.02	1.02 =	C8H8N2O4	N-METHYL-2-NITROPHENYLCARBAMATE
2741	OCTANOL	384		1.39	1.39 =	C8H8N2O4	N-METHYL-3-NITROPHENYLCARBAMATE
2742	OCTANOL	384		1.47	1.47 =	C8H8N2O4	N-METHYL-4-NITROPHENYLCARBAMATE
2743	OCTANOL	10		1.58	1.58 =	C8H8O1	ACETOPHENONE
2744	DIETHYL ETHER	248	50	1.75	1.67 A	C8H8O1	ACETOPHENONE
2745	BENZENE	248	12	2.20	2.07 B	C8H8O1	ACETOPHENONE
2746	CLCH2CH2CL	248		2.38		C8H8O1	ACETOPHENONE
2747	OCTANOL	268		2.23	2.23 =	C8H8O1S1	THIOACETIC ACID, S-PHENYL ESTER
2748	OCTANOL	10		1.49	1.49 =	C8H8O2	ACETIC ACID, PHENYL ESTER
2749	OCTANOL	10		1.39	1.39 =	C8H8O2	M-ACETYLPHENOL
2750	OCTANOL	10		1.35	1.35 =	C8H8O2	P-ACETYLPHENOL
2751	CYCLOHEXANE	56		-2.14		C8H8O2	P-ACETYLPHENOL
2752	OCTANOL	10		2.12	2.12 =	C8H8O2	BENZOIC ACID,METHYL ESTER
2753	OCTANOL	10		1.41	1.41 =	C8H8O2	PHENYLACETIC ACID
2754	DIETHYL ETHER	3		1.57	1.49 A	C8H8O2	PHENYLACETIC ACID
2755	DIETHYL ETHER	207		1.33	1.28 A	C8H8O2	PHENYLACETIC ACID
2756	DIETHYL ETHER	46		1.44	1.37 A	C8H8O2	PHENYLACETIC ACID
2757	CHCL3	29	12	0.45	1.63 A	C8H8O2	PHENYLACETIC ACID
2758	OILS	361		0.35	1.57 A	C8H8O2	PHENYLACETIC ACID
2759	OILS	362		0.13	1.33 A	C8H8O2	PHENYLACETIC ACID
2760	OILS	385		0.26	1.42 A	C8H8O2	PHENYLACETIC ACID
2761	BENZENE	29		-0.03	1.38 A	C8H8O2	PHENYLACETIC ACID
2762	I-BUTANOL	4		1.43	1.51	C8H8O2	PHENYLACETIC ACID
2763	XYLENE	46		-0.38	1.38 A	C8H8O2	PHENYLACETIC ACID
2764	TOLUENE	48		0.09	1.66 A	C8H8O2	PHENYLACETIC ACID
2765	TOLUENE	29		-0.13	1.46 A	C8H8O2	PHENYLACETIC ACID
2766	NITROBENZENE	48		0.67	1.42	C8H8O2	PHENYLACETIC ACID
2767	PRIM. PENTANOLS	48		1.48	1.57	C8H8O2	PHENYLACETIC ACID
2768	OCTANOL	10		2.37	2.37 =	C8H8O2	M-TOLUIC ACID
2769	CYCLOHEXANE	357		0.65		C8H8O2	O-TOLUIC ACID
2770	CHCL3	29	25	1.76	2.83 A	C8H8O2	O-TOLUIC ACID
2771	TOLUENE	29		1.10	2.54 A	C8H8O2	O-TOLUIC ACID
2772	OCTANOL	10		2.27	2.27 =	C8H8O2	P-TOLUIC ACID
2773	CHCL3	29	12	1.81	2.91 A	C8H8O2	P-TOLUIC ACID
2774	TOLUENE	29		0.68	2.18 A	C8H8O2	P-TOLUIC ACID
2775	OCTANOL	386		1.91	1.91 =	C8H8O2S1	PHENYLTHIO-ACETIC ACID
2776	BENZENE	279		2.40	3.70 A	C8H8O2S1	THENOYLACETONE
2777	CCL4	279		2.06	3.57 N	C8H8O2S1	THENOYLACETONE
2778	HEXANE	279		1.30		C8H8O2S1	THENOYLACETONE
2779	O-DICL. BENZENE	279		2.49		C8H8O2S1	THENOYLACETONE
2780	OCTANOL	386		2.05	2.05 =	C8H8O2SE1	PHENYLSELENO-ACETIC ACID
2781	CHCL3	387		2.92	3.89 A	C8H8O2SE1	1-(2-SELENOPHEN-YL)-1,3-BUTANEDIONE
2782	CHCL3	388		3.39	4.30 A	C8H8O2SE1	1-(2-SELENOPHEN-YL)-1,3-BUTANEDIONE
2783	BENZENE	387		3.00	4.30 A	C8H8O2SE1	1-(2-SELENOPHEN-YL)-1,3-BUTANEDIONE
2784	BENZENE	388		2.92	4.23 A	C8H8O2SE1	1-(2-SELENOPHEN-YL)-1,3-BUTANEDIONE
2785	DIETHYL ETHER	323		1.35	1.30 A	C8H8O3	BENZALDEHYDE,2-HYDROXY-3-METHOXY/O-VANILLIN/
2786	DIETHYL ETHER	3		0.97	0.96 A	C8H8O3	BENZALDEHYDE,3-METHOXY,4-HYDROXY/VANILLIN/
2787	DIETHYL ETHER	323		0.91	0.91 A	C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2788	DIETHYL ETHER	359		0.93	0.94 A	C8H8O3	BENZALDEHYDE,3-METHOXY,4-HYDROXY/VANILLIN/
2789	DIETHYL ETHER	248		0.96	0.96 A	C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2790	CYCLOHEXANE	248		-0.75		C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2791	CHCL3	366		1.42	1.92 N	C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2792	OILS	173		0.42	1.58 A	C8H8O3	BENZALDEHYDE,3-METHOXY,4-HYDROXY/VANILLIN/
2793	OILS	224		0.48	1.63 A	C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2794	BENZENE	389		0.81	2.20 A	C8H8O3	BENZALDEHYDE,3-METHOXY,4-HYDROXY/VANILLIN/
2795	BENZENE	248		0.82	2.21 A	C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2796	TOLUENE	389		0.64	2.14 A	C8H8O3	BENZALDEHYDE,3-METHOXY,4-HYDROXY/VANILLIN/
2797	CLCH2CH2CL	248		1.29		C8H8O3	BENZALDEHYDE,3-METHOXY-4-HYDROXY/VANILLIN/
2798	DI-I-PR. ETHER	366		0.60	1.24	C8H8O3	BENZALDEHYDE,3-METHOXY,4-HYDROXY/VANILLIN/
2799	OCTANOL	186		1.05	1.05 =	C8H8O3	BENZYL ALCOHOL,3,4-METHYLENEDIOXY
2800	OCTANOL	261		1.89	1.89 =	C8H8O3	M-CARBOMETHOXYPHENOL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
2801	OCTANOL	261		1.96	1.96 =	C8H8O3	P-CARBOMETHOXYPHENOL
2802	OCTANOL	235		1.96	1.96 =	C8H8O3	P-HYDROXYBENZOIC ACID, METHYL ESTER
2803	OCTANOL	10		0.85	0.85 =	C8H8O3	M-HYDROXYPHENYLACETIC ACID
2804	OCTANOL	10		0.85	0.85 =	C8H8O3	O-HYDROXYPHENYLACETIC ACID
2805	OILS	383		-1.04	0.27 A	C8H8O3	P-HYDROXYPHENYLACETIC ACID
2806	OCTANOL	10		2.02	2.02 =	C8H8O3	M-METHOXYBENZOIC ACID
2807	DIETHYL ETHER	112		0.78	0.80 A	C8H8O3	O-METHOXYBENZOIC ACID
2808	CHCL3	112		1.65	2.72 A	C8H8O3	O-METHOXYBENZOIC ACID
2809	CHCL3	29		1.65	2.93 A	C8H8O3	O-METHOXYBENZOIC ACID
2810	BENZENE	17		0.64	2.02 A	C8H8O3	O-METHOXYBENZOIC ACID
2811	TOLUENE	29		0.45	1.97 A	C8H8O3	O-METHOXYBENZOIC ACID
2812	OCTANOL	10		1.96	1.96 =	C8H8O3	P-METHOXYBENZOIC ACID/ANISIC ACID/
2813	CHCL3	29	12	1.48	2.56 A	C8H8O3	P-METHOXYBENZOIC ACID/ANISIC ACID/
2814	CHCL3	46		0.90	2.04 A	C8H8O3	P-METHOXYBENZOIC ACID/ANISIC ACID/
2815	BENZENE	17		0.46	1.85 A	C8H8O3	P-METHOXYBENZOIC ACID/ANISIC ACID/
2816	XYLENE	46		-0.26	1.51 A	C8H8O3	P-METHOXYBENZOIC ACID/ANISIC ACID/
2817	TOLUENE	29		0.54	2.05 A	C8H8O3	P-METHOXYBENZOIC ACID/ANISIC ACID/
2818	OCTANOL	10		1.26	1.26 =	C8H8O3	PHENOXYACETIC ACID
2819	CYCLOHEXANONE	302		2.18		C8H8O3	PHENOXYACETIC ACID
2820	ME-I-BUT.KETONE	302		1.54		C8H8O3	PHENOXYACETIC ACID
2821	CYCLOHEXANOL	302		1.61		C8H8O3	PHENOXYACETIC ACID
2822	DIETHYL ETHER	3		0.35	0.42 A	C8H8O3	PHENYLACETIC ACID,A-HYDROXY/MANDELIC ACID/
2823	DIETHYL ETHER	207		0.30	0.38 A	C8H8O3	PHENYLACETIC ACID,A-HYDROXY/MANDELIC ACID/
2824	DIETHYL ETHER	46		0.28	0.37 A	C8H8O3	PHENYLACETIC ACID,A-HYDROXY/MANDELIC ACID/
2825	CHCL3	29		-1.26	0.07 A	C8H8O3	PHENYLACETIC ACID,A-HYDROXY/MANDELIC ACID/
2826	BENZENE	36	12	-1.95	-0.54 A	C8H8O3	PHENYLACETIC ACID,A-HYDROXY/MANDELIC ACID/
2827	I-BUTANOL	4		0.72	0.50	C8H8O3	PHENYLACETIC ACID,A-HYDROXY/MANDELIC ACID/
2828	OCTANOL	10		0.76	0.76 =	C8H8O4	PHENOXYACETIC ACID,M-HYDROXY
2829	OCTANOL	302		0.85	0.85 =	C8H8O4	PHENOXYACETIC ACID,O-HYDROXY
2830	OCTANOL	10		0.65	0.65 =	C8H8O4	PHENOXYACETIC ACID,P-HYDROXY
2831	CYCLOHEXANONE	302		1.91		C8H8O4	PHENOXYACETIC ACID,P-HYDROXY
2832	ME-I-BUT.KETONE	302		1.05		C8H8O4	PHENOXYACETIC ACID,P-HYDROXY
2833	CYCLOHEXANOL	302		1.32		C8H8O4	PHENOXYACETIC ACID,P-HYDROXY
2834	OCTANOL	255		3.09	3.09 =	C8H9BR1	BENZENE,2-BROMO-1-ETHYL
2835	OCTANOL	255		2.95	2.95 =	C8H9CL1	BENZENE,2-CHLORO-1-ETHYL
2836	OCTANOL	10		1.16	1.16 =	C8H9N1O1	ACETANILIDE
2837	DIETHYL ETHER	3		0.48	1.28 B	C8H9N1O1	ACETANILIDE
2838	DIETHYL ETHER	359		0.50	1.29 B	C8H9N1O1	ACETANILIDE
2839	CHCL3	359		0.89	1.41 N	C8H9N1O1	ACETANILIDE
2840	CHCL3	254		0.88	1.39 N	C8H9N1O1	ACETANILIDE
2841	CHCL3	338	44	0.48	1.06 N	C8H9N1O1	ACETANILIDE
2842	OILS	173		0.00	1.19 A	C8H9N1O1	ACETANILIDE
2843	OILS	224		0.30	1.47 A	C8H9N1O1	ACETANILIDE
2844	BENZENE	338	44	-1.70		C8H9N1O1	ACETANILIDE
2845	BENZENE	72		0.22	1.59 A	C8H9N1O1	ACETANILIDE
2846	N-HEPTANE	254		-1.70		C8H9N1O1	ACETANILIDE
2847	N-HEPTANE	338	44	-2.00		C8H9N1O1	ACETANILIDE
2848	TOLUENE	151		1.77	3.13 A	C8H9N1O1	N-METHYL-SALICYLIDENEIMINE /SCHIFF BASE/
2849	CYCLOHEXANE	151		0.95		C8H9N1O1	N-METHYL-SALICYLIDINEIMINE /SCHIFF BASE/
2850	OCTANOL	255		0.45	0.45 =	C8H9N1O1	PHENYLACETAMIDE
2851	OLEYL ALCOHOL	390	44	1.09	1.63	C8H9N1O2	P-AMINOBENZOIC ACID,METHYL ESTER
2852	OILS	383		-0.89	0.40 A	C8H9N1O2	P-AMINOPHENYLACETIC ACID
2853	CHCL3	29		0.81	1.98 A	C8H9N1O2	ANTHRANILIC ACID,N-METHYL
2854	TOLUENE	29		0.61	2.11 A	C8H9N1O2	ANTHRANILIC ACID,N-METHYL
2855	CYCLOHEXANE	141		1.81		C8H9N1O2	BENZENE,B-NITROETHYL
2856	OCTANOL	65		2.95	2.95 =	C8H9N1O2	1,3-DIMETHYL-2-NITROBENZENE
2857	OCTANOL	386		0.62	0.62 =	C8H9N1O2	GLYCINE, N-PHENYL
2858	OCTANOL	276		0.94	0.94 =	C8H9N1O2	M-METHOXYBENZAMIDE
2859	OCTANOL	276		0.87	0.87 =	C8H9N1O2	O-METHOXYBENZAMIDE
2860	OCTANOL	276		0.86	0.86 =	C8H9N1O2	P-METHOXYBENZAMIDE
2861	OCTANOL	384		1.16	1.16 =	C8H9N1O2	N-METHYLPHENYLCARBAMATE
2862	OCTANOL	186		1.24	1.24 =	C8H9N1O2	N-METHYLPHENYLCARBAMATE
2863	HEXANE	391		-0.54		C8H9N1O2	N-METHYLPHENYLCARBAMATE
2864	OCTANOL	349		1.32	1.32 =	C8H9N1O2	NICOTINIC ACID, ETHYL ESTER
2865	OCTANOL	349		1.43	1.43 =	C8H9N1O2	I-NICOTINIC ACID, ETHYL ESTER
2866	OCTANOL	349		0.87	0.87 =	C8H9N1O2	PICOLINIC ACID, ETHYL ESTER
2867	OILS	381		-0.01	1.18 A	C8H9N1O2	TETRAHYDROPHTHALIMIDE
2868	N-HEPTANE	370	14	0.28		C8H9N1O3	P-AMINOSALICYLIC ACID,METHYL ESTER
2869	OILS	249		0.25	1.41 A	C8H9N1O3	ORTHOCAINE
2870	CYCLOHEXANONE	302		0.71		C8H9N1O3	PHENOXYACETIC ACID,P-AMINO
2871	OCTANOL	217	07	0.20	0.20 =	C8H9N1O3S1	P-ACETYLBENZENESULFONAMIDE
2872	CHCL3	217	07	-0.36	0.24 N	C8H9N1O3S1	P-ACETYLBENZENESULFONAMIDE
2873	OCTANOL	276		1.61	1.61 =	C8H9N3O1S1	M-HYDROXYBENZYLIDINETHIOUREA
2874	OCTANOL	226		-0.57	-0.57 =	C8H9N3O2	1-ACETYL-2-PICOLINOYLHYDRAZINE (68626)
2875	OCTANOL	255		3.15	3.15 =	C8H10	BENZENE,ETHYL
2876	OCTANOL	301		3.20	3.20 =	C8H10	M-XYLENE
2877	N-HEPTANE	310		3.54		C8H10	M-XYLENE
2878	OCTANOL	301		2.77	2.77 =	C8H10	O-XYLENE
2879	N-HEPTANE	310		3.39		C8H10	O-XYLENE
2880	OCTANOL	301		3.15	3.15 =	C8H10	P-XYLENE
2881	N-HEPTANE	310		3.45		C8H10	P-XYLENE
2882	OCTANOL	80		1.71	1.71 =	C8H10CL1N1O2	O-(1-ETHYL-1-ETHYNYL-3-CHLOROALLYL)CARBAMATE
2883	OCTANOL	392		2.04	2.04 =	C8H10N1O5P1S1	DIMETHYLPARATHION
2884	CHCL3	392		1.38	0.97 B	C8H10N1O5P1S1	DIMETHYLPARATHION
2885	BENZENE	392		1.28	1.44 B	C8H10N1O5P1S1	DIMETHYLPARATHION
2886	OCTANOL	392		1.33	1.33 =	C8H10N1O6P1	DIMETHYLPARA-OXON
2887	CHCL3	392		1.33	0.91 B	C8H10N1O6P1	DIMETHYLPARA-OXON
2888	BENZENE	392		1.17	1.36 B	C8H10N1O6P1	DIMETHYLPARA-OXON
2889	BENZENE	72		1.71	1.73 B	C8H10N2O1	P-NITROSODIMETHYLANILINE
2890	OCTANOL	186		0.42	0.42 =	C8H10N2O1	UREA,1-METHYL-1-PHENYL
2891	DIETHYL ETHER	113	15	-0.67	-0.47 A	C8H10N2O3S1	SULFANILACETAMIDE
2892	CHCL3	343	2	-0.66	-0.01 N	C8H10N2O3S1	SULFANILACETAMIDE
2893	CHCL3	113	15	-0.12	0.48 N	C8H10N2O3S1	SULFANILACETAMIDE
2894	CHCL3	393	63	-0.35	0.27 N	C8H10N2O3S1	SULFANILACETAMIDE
2895	BENZENE	343	2	-1.54	-0.14 A	C8H10N2O3S1	SULFANILACETAMIDE
2896	1-PENT. ACETATE	343	2	-0.06	-0.24	C8H10N2O3S1	SULFANILACETAMIDE
2897	CCL4	343	2	-1.77	-1.72 N	C8H10N2O3S1	SULFANILACETAMIDE
2898	OCTANOL	186		0.85	0.85 =	C8H10N2S1	UREA,1-METHYL-1-PHENYL-2-THIO
2899	OCTANOL	218		-0.07	-0.07 =	C8H10N4O2	CAFFEINE
2900	DIETHYL ETHER	3		-1.30	-0.30 B	C8H10N4O2	CAFFEINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT		EMPIRICAL FORMULA	NAME
2901	CHCL3	394	42	1.33	0.91	B	C8H10N402	CAFFEINE
2902	CHCL3	359	42	1.32	0.86	B	C8H10N402	CAFFEINE
2903	CHCL3	322	42	1.28	0.87	B	C8H10N402	CAFFEINE
2904	OILS	371		-0.40	0.18	B	C8H10N402	CAFFEINE
2905	OILS	2	12	-1.48	-0.79	B	C8H10N402	CAFFEINE
2906	OILS	249		-1.13	-0.50	B	C8H10N402	CAFFEINE
2907	1-BUTANOL	4		0.08	-0.39		C8H10N402	CAFFEINE
2908	I-PENT. ACETATE	395	14	-2.22			C8H10N402	CAFFEINE
2909	CCL4	234	12	-0.68			C8H10N402	CAFFEINE
2910	BENZENE	368	68	-0.16	0.44	B	C8H10N402	CAFFIENE
2911	OCTANOL	206	27	3.58	3.58	=	C8H10N406S3	PURINE, 2,6,8-TRI-METHYLSULFONYL
2912	CYCLOHEXANE	325		0.51			C8H1001	2,3-DIMETHYLPHENOL
2913	N-HEPTANE	310		0.43			C8H1001	2,3-DIMETHYLPHENOL
2914	CYCLOHEXANE	132		0.76			C8H1001	2,4-DIMETHYLPHENOL
2915	CYCLOHEXANE	325		0.55			C8H1001	2,4-DIMETHYLPHENOL
2916	N-HEPTANE	310		0.40			C8H1001	2,4-DIMETHYLPHENOL
2917	CYCLOHEXANE	132		0.77			C8H1001	2,5-DIMETHYLPHENOL
2918	CYCLOHEXANE	325		0.57			C8H1001	2,5-DIMETHYLPHENOL
2919	N-HEPTANE	310		0.52			C8H1001	2,5-DIMETHYLPHENOL
2920	OCTANOL	261		2.36	2.36	=	C8H1001	2,6-DIMETHYLPHENOL
2921	DIETHYL ETHER	323		2.53	2.33	A	C8H1001	2,6-DIMETHYLPHENOL
2922	CYCLOHEXANE	132		1.28			C8H1001	2,6-DIMETHYLPHENOL
2923	CYCLOHEXANE	325		0.93			C8H1001	2,6-DIMETHYLPHENOL
2924	N-HEPTANE	310		0.82			C8H1001	2,6-DIMETHYLPHENOL
2925	CYCLOHEXANE	325		0.20			C8H1001	3,4-DIMETHYLPHENOL
2926	N-HEPTANE	310		0.10			C8H1001	3,4-DIMETHYLPHENOL
2927	OCTANOL	261		2.35	2.35	=	C8H1001	3,5-DIMETHYLPHENOL
2928	CYCLOHEXANE	132		0.54			C8H1001	3,5-DIMETHYLPHENOL
2929	CYCLOHEXANE	325		0.27			C8H1001	3,5-DIMETHYLPHENOL
2930	N-HEPTANE	310		0.21			C8H1001	3,5-DIMETHYLPHENOL
2931	OCTANOL	255		1.36	1.36	=	C8H1001	ETHANOL,2-PHENYL
2932	HEXANE	372		-0.39			C8H1001	ETHANOL,2-PHENYL
2933	OCTANOL	10		2.40	2.40	=	C8H1001	M-ETHYLPHENOL
2934	CYCLOHEXANE	132		0.43			C8H1001	M-ETHYLPHENOL
2935	CYCLOHEXANE	325		0.36			C8H1001	M-ETHYLPHENOL
2936	CYCLOHEXANE	132		0.83			C8H1001	O-ETHYLPHENOL
2937	CYCLOHEXANE	325		0.68			C8H1001	O-ETHYLPHENOL
2938	CYCLOHEXANE	132		0.44			C8H1001	P-ETHYLPHENOL
2939	CYCLOHEXANE	325		0.37			C8H1001	P-ETHYLPHENOL
2940	OILS	324	12	1.79	2.81	A	C8H1001	P-ETHYLPHENOL
2941	OILS	327		1.62	2.66	A	C8H1001	P-ETHYLPHENOL
2942	BENZENE	324	45	1.44	2.78	A	C8H1001	P-ETHYLPHENOL
2943	PARAFFINS	327		0.04			C8H1001	P-ETHYLPHENOL
2944	OCTANOL	10		1.60	1.60	=	C8H1001	M-METHYLBENZYL ALCOHOL
2945	OCTANOL	10		1.58	1.58	=	C8H1001	P-METHYLBENZYL ALCOHOL
2946	CYCLOHEXANE	358		2.77			C8H1001	PHENETOLE
2947	DIETHYL ETHER	332		1.65	1.57	A	C8H1002	BENZENE,1,2-DIHYDROXY-4-ETHYL
2948	DI-BUTYL ETHER	332		0.88			C8H1002	BENZENE,1,2-DIHYDROXY,4-ETHYL
2949	DI-I-PR. ETHER	332		1.39	2.16		C8H1002	BENZENE,1,2-DIHYDROXY,4-ETHYL
2950	CYCLOHEXANE	358		2.32			C8H1002	BENZENE,1,3-DIMETHOXY
2951	OILS	173		2.15	3.14	A	C8H1002	BENZENE,1,4-DIMETHOXY
2952	OILS	224		2.21	3.20	A	C8H1002	BENZENE,1,4-DIMETHOXY
2953	OCTANOL	261		1.81	1.81	=	C8H1002	P-ETHOXYPHENOL
2954	OCTANOL	10		1.10	1.10	=	C8H1002	P-METHOXYBENZYL ALCOHOL
2955	OILS	327		1.26	2.33	A	C8H1002	PHENOL,2-METHOXY-4-METHYL/P-METHYLGUAIACOL/
2956	PARAFFINS	327		0.71			C8H1002	PHENOL,2-METHOXY-4-METHYL/P-METHYLGUAIACOL/
2957	OCTANOL	56		1.16	1.16	=	C8H1002	2-PHENOXYETHANOL
2958	N-BUTYL ACETATE	331		1.21	1.26		C8H1002	RESORCINOL,4,5-DIMETHYL
2959	N-BUTYL ACETATE	331		1.64	1.62		C8H1002	RESORCINOL,2,4-DIMETHYL
2960	N-BUTYL ACETATE	331		1.94	1.82		C8H1002	RESORCINOL,2,5-DIMETHYL
2961	DIETHYL ETHER	323		-0.20	-0.06	A	C8H1003	BENZYL ALCOHOL,4-HYDROXY,3-METHOXY
2962	DIETHYL ETHER	323		0.74	0.76	A	C8H1003	PHENOL,2,6-DIMETHOXY
2963	OILS	327		0.57	1.69	A	C8H1003	PHENOL,2,6-DIMETHOXY
2964	PARAFFINS	327		-0.36			C8H1003	PHENOL,2,6-DIMETHOXY
2965	BENZENE	311	6	-0.01			C8H11B103	P-ETHOXYPHENYLBORONIC ACID
2966	OCTANOL	373		-2.02	-2.02	=	C8H11CL1N201	N1-ETHYLNICOTINAMIDE CHLORIDE
2967	DIETHYL ETHER	46		0.78	1.54	B	C8H11N1	BENZYLMETHYLAMINE
2968	DIETHYL ETHER	374		0.85	1.61	B	C8H11N1	BENZYLMETHYLAMINE
2969	XYLENE	46		1.39	2.03	B	C8H11N1	BENZYLMETHYLAMINE
2970	OCTANOL	10		2.31	2.31	=	C8H11N1	N,N-DIMETHYLANILINE
2971	OCTANOL	309		2.62	2.62	=	C8H11N1	N,N-DIMETHYLANILINE
2972	CYCLOHEXANE	337		2.47			C8H11N1	N,N-DIMETHYLANILINE
2973	N-HEPTANE	310		1.00			C8H11N1	2,3-DIMETHYLANILINE
2974	CYCLOHEXANE	337		1.23			C8H11N1	2,4-DIMETHYLANILINE
2975	XYLENE	46		1.18	1.85	B	C8H11N1	2,4-DIMETHYLANILINE
2976	N-HEPTANE	310		1.10			C8H11N1	2,4-DIMETHYLANILINE
2977	CYCLOHEXANE	337		1.22			C8H11N1	2,5-DIMETHYLANILINE
2978	N-HEPTANE	310		1.12			C8H11N1	2,5-DIMETHYLANILINE
2979	CYCLOHEXANE	337		1.35			C8H11N1	2,6-DIMETHYLANILINE
2980	N-HEPTANE	310		1.21			C8H11N1	2,6-DIMETHYLANILINE
2981	XYLENE	46		1.05	1.70	B	C8H11N1	3,4-DIMETHYLANILINE
2982	N-HEPTANE	310		0.95			C8H11N1	3,4-DIMETHYLANILINE
2983	CYCLOHEXANE	337		1.18			C8H11N1	3,5-DIMETHYLANILINE
2984	OCTANOL	255		1.41	1.41	=	C8H11N1	ETHYLAMINE,2-PHENYL
2985	CHCL3	396	31	1.32	0.91	B	C8H11N1	ETHYLAMINE,2-PHENYL
2986	N-HEPTANE	396	31	-0.56			C8H11N1	ETHYLAMINE,2-PHENYL
2987	OCTANOL	312		2.26	2.26	=	C8H11N1	N-ETHYLANILINE
2988	XYLENE	73		1.72	2.36	B	C8H11N1	PYRIDINE,2-METHYL,5-ETHYL
2989	TOLUENE	73		1.80	1.95	B	C8H11N1	PYRIDINE,2-METHYL,5-ETHYL
2990	OCTANOL	9		2.10	2.10	=	C8H11N1	PYRIDINE,4-PROPYL
2991	TOLUENE	188		1.43	1.72	B	C8H11N1	PYRIDINE,2,4,6-TRIMETHYL/COLLIDIN/
2992	OCTANOL	10		1.56	1.56	=	C8H11N101	3-DIMETHYLAMINOPHENOL
2993	OCTANOL	80		1.09	1.09	=	C8H11N102	O-(1-ETHYL-1-VINYL-2-PROPYNYL) CARBAMATE
2994	OILS	381		0.16	1.34	A	C8H11N102	HEXAHYDROPHTHALIMIDE
2995	DIETHYL ETHER	113		1.11	1.09	A	C8H11N102S1	BENZENESULFONAMIDE,N-ETHYL
2996	CHCL3	113		1.77	2.28	N	C8H11N102S1	BENZENESULFONAMIDE,N-ETHYL
2997	DIETHYL ETHER	113		1.16	1.13	A	C8H11N102S1	N,N-DIMETHYLBENZENESULFONAMIDE
2998	CHCL3	113		2.69	3.11	N	C8H11N102S1	N,N-DIMETHYLBENZENESULFONAMIDE
2999	OCTANOL	227		-2.14	-2.14	=	C8H11N306	6-AZAURIDINE (NCS 32074)(PKA= 6.63)
3000	OCTANOL	397		0.74	0.74	=	C8H11N5	ADENINE,9-PROPYL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3001	OCTANOL	341	60	0.49	0.49 =	C8H12N2	N,N-DIMETHYL-3-PYRIDYLMETHYLAMINE
3002	OCTANOL	341	60	0.76	0.76 =	C8H12N2	N-ETHYL-3-PYRIDYLMETHYLAMINE
3003	CHCL3	322		0.88	1.36 N	C8H12N2O1S1	2-METHIO-4-HYDROXYTRIMETHYLENEPYRIMIDINE
3004	OCTANOL	56		0.81	0.81 =	C8H12N2O2S1	PHENETHYL SULFAMIDE
3005	OILS	398	44	0.36	1.52 A	C8H12N2O2S1	2-THIO-5,5-DIETHYLBARBITURIC ACID/THIOBARBITAL/
3006	OCTANOL	80		0.65	0.65 =	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3007	DIETHYL ETHER	113	16	0.63	0.67 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3008	CHCL3	399	1	-0.14	0.49 N	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3009	CHCL3	113		-0.07	0.54 N	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3010	CHCL3	254		-0.15	0.45 N	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3011	CHCL3	338	44	0.45	1.03 N	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3012	OILS	82		-0.72	0.54 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3013	OILS	345		-0.67	0.58 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3014	OILS	398	44	-0.58	0.68 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3015	OILS	296	12	-1.22	0.08 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3016	OILS	168		-0.57	0.69 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3017	OILS	290		-0.96	0.32 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3018	BENZENE	399	1	-0.77	0.62 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3019	BENZENE	338	44	-1.85		C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3020	I-PENT. ACETATE	399	1	0.58	0.43	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3021	CCL4	399	1	-1.46	0.62 A	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3022	N-HEPTANE	338	44	-2.15		C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3023	OLEYL ALCOHOL	82		0.14	0.70	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3024	50%ETHER+50%DMF	125		-0.10	0.55	C8H12N2O3	5,5-DIETHYLBARBITURIC ACID/BARBITAL/VERONAL/
3025	OCTANOL	80		1.73	1.73 =	C8H12O1	CYCLOHEXANOL,1-ETHYNYL
3026	DIETHYL ETHER	112		0.29	0.37 A	C8H12O2	CYCLOHEXANE-1,3-DIONE,5,5-DIMETHYL/DIMEDON/
3027	CHCL3	112		0.76	1.30 N	C8H12O2	CYCLOHEXANE-1,3-DIONE,5,5-DIMETHYL/DIMEDON/
3028	OILS	347		1.42	2.48 A	C8H12O2	SORBIC ACID,ETHYL ESTER
3029	OCTANOL	298		3.99	3.99 =	C8H12SI1	SILANE, DIMETHYL-PHENYL
3030	N-HEPTANE	400	14	-1.15		C8H13N1O2	ARECOLIN
3031	OCTANOL	348		-0.04	-0.04 =	C8H13N1O2	N-PROPIONYLCYCLOBUTANECARBOXAMIDE
3032	OCTANOL	218		1.52	1.52 =	C8H13N1O2S1	3,5-THIOMORPHOLINEDIONE,2,2-DIETHYL
3033	OCTANOL	134		1.52	1.52 =	C8H14N4O1S1	3-ETHYLTHIO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
3034	OCTANOL	134		1.39	1.39 =	C8H14N4O1S1	3-METHIO-4-AMINO-6-I-BU-1,2,4-TRIAZINE-5-ONE
3035	OCTANOL	134		1.70	1.70 =	C8H14N4O1S1	3-METHIO-4-AMINO-6-T-BU-1,2,4-TRIAZINE-5-ONE
3036	CHCL3	285		2.97	4.20 A	C8H14O2	6-METHYL-2,4-HEPTANEDIONE/I-VALERYLACETONE/
3037	OCTANOL	255		0.55	0.55 =	C8H14O3	HEPTANOIC ACID, 6-KETO METHYL ESTER
3038	DIETHYL ETHER	212		0.67	0.70 A	C8H14O4	SUBERIC ACID
3039	DIETHYL ETHER	194		0.47	0.54 A	C8H14O4	SUBERIC ACID
3040	N-BUTANOL	194		0.92	0.80	C8H14O4	SUBERIC ACID
3041	ETHYL ACETATE	194		0.70	0.70	C8H14O4	SUBERIC ACID
3042	CYCLOHEXANONE	194		0.85		C8H14O4	SUBERIC ACID
3043	2-BUTANONE	194		0.68	0.72	C8H14O4	SUBERIC ACID
3044	ME-I-BUT.KETONE	194		0.68	0.74	C8H14O4	SUBERIC ACID
3045	OCTANOL	56		-0.29	-0.29 =	C8H14O6	TARTARIC ACID,DIETHYL ESTER
3046	DIETHYL ETHER	3		-0.19	-0.05 A	C8H14O6	TARTARIC ACID,DIETHYL ESTER
3047	DIETHYL ETHER	401		-0.35	-0.19 A	C8H14O6	TARTARIC ACID,DIETHYL ESTER
3048	1-OCTANOL	353		-1.38		C8H15K1O2	POTASSIUM OCTANOATE
3049	OCTANOL	260		0.67	0.67 =	C8H15N1O1	2-AZACYCLONONANONE
3050	DIETHYL ETHER	3		-1.28	-0.28 B	C8H15N1O1	TROPINE
3051	I-BUTANOL	4		0.49	0.21	C8H15N1O1	TROPINE
3052	CHCL3	67		-0.77		C8H15N1O3	D-ISOLEUCINE,ACETYL
3053	CHCL3	67		-0.84		C8H15N1O3	D-LEUCINE,ACETYL
3054	CHCL3	67		-0.70		C8H15N1O3	NORLEUCINE,ACETYL
3055	OCTANOL	260		1.44	1.44 =	C8H15N1S1	2-AZACYCLONONANTHIONE
3056	OCTANOL	227		-1.45	-1.45 =	C8H15N3O7	STREPTOZOTOCIN (NCS 85998)
3057	1-OCTANOL	353		-1.38		C8H15NA1O2	SODIUM OCTANOATE
3058	PARAFFINS	241		-0.57		C8H16N2S1	N-AMYLETHYLENETHIOUREA
3059	N-HEPTANE	139	31	0.63		C8H16O2	OCTANOIC ACID
3060	CHCL3	402	46	-0.92		C8H17CL2N1O2	DI-I-PROPYLAMMONIUM-DICHLOROACETATE
3061	BENZENE	402	46	-1.77		C8H17CL2N1O2	DI-I-PROPYLAMMONIUM-DICHLOROACETATE
3062	I-BUTANOL	4		1.99	2.29	C8H17N1	2-PROPYLPIPERIDINE/CONIINE/
3063	XYLENE	46		1.95	2.61 B	C8H17N1	2-PROPYLPIPERIDINE/CONIINE/
3064	OCTANOL	218		1.81	1.81 =	C8H17N1O1S1	PROPIONAMIDE,2-BUTYLTHIO-2-METHYL
3065	OILS	271		1.79	1.92 B	C8H18F1O3P1	DIBUTYLFLUOROPHOSPHATE
3066	CCL4	271		2.01	1.77 B	C8H18F1O3P1	DIBUTYLFLUOROPHOSPHATE
3067	DIETHYL ETHER	378	44	-1.00	0.06 B	C8H18N2O2	N-METHYLCARBAMIC ACID,DIETHYLAMINOETHYL ESTER
3068	OCTANOL	5		3.15	3.15 =	C8H18O1	OCTANOL
3069	OILS	201		1.77	2.80 A	C8H18O1	OCTANOL
3070	DIETHYL ETHER	2		0.04	0.15 A	C8H18O3	DIETHYLENE GLYCOL,MONOBUTYL ETHER
3071	OILS	2		-0.92	0.40 A	C8H18O3	DIETHYLENE GLYCOL,MONOBUTYL ETHER
3072	OILS	173		0.72	1.04 B	C8H18O4S2	2,2-BIS(ETHYLSULFONYL)BUTANE/TRIONAL/
3073	OILS	168		0.66	0.98 B	C8H18O4S2	2,2-BIS(ETHYLSULFONYL)BUTANE/TRIONAL/
3074	OILS	214		0.65	0.97 B	C8H18O4S2	2,2-BIS(ETHYLSULFONYL)BUTANE/TRIONAL/
3075	DIETHYL ETHER	3		-2.62	-2.18 A	C8H18O5	TETRAETHYLENE GLYCOL
3076	1-BUTANOL	4		-0.62	-1.38	C8H18O5	TETRAETHYLENE GLYCOL
3077	DIETHYL ETHER	3		2.52	3.04 B	C8H19N1	DI-1-BUTYLAMINE
3078	1-BUTANOL	4		2.38	2.84	C8H19N1	DI-I-BUTYLAMINE
3079	OCTANOL	218		2.68	2.68 =	C8H19N1	DIBUTYLAMINE
3080	I-BUTANOL	4		2.35	2.90	C8H19N1	OCTYLAMINE
3081	CCL4	135		2.63	2.33 B	C8H19O2P1S2	PHOSPHORODITHIOTIC ACID,DI-1-BUTYL
3082	I-PENT. ACETATE	135		2.23	2.13	C8H19O2P1S2	PHOSPHORODITHIOTIC ACID,DI-N-BUTYL
3083	CCL4	135		2.52	2.26 B	C8H19O2P1S2	PHOSPHORODITHIOTIC ACID,DI-N-BUTYL
3084	ME-I-BUT.KETONE	135		2.54	2.27	C8H19O2P1S2	PHOSPHORODITHIOTIC ACID,DI-N-BUTYL
3085	OCTANOL	56		2.03	2.03 =	C8H19O2S2	ETHYLPHOSPHONATE,O-ET-S-(2-ET-THIOETHYL)
3086	DI-BUTYL ETHER	236	17	1.04		C8H19O4P1	DI-I-BUTYL PHOSPHATE
3087	CHCL3	50		0.24	1.44 A	C8H19O4P1	DIBUTYL PHOSPHATE
3088	CHCL3	403		0.34	1.53 A	C8H19O4P1	DIBUTYL PHOSPHATE
3089	BENZENE	50		-0.42		C8H19O4P1	DIBUTYL PHOSPHATE
3090	BENZENE	404		-0.42	1.00 A	C8H19O4P1	DIBUTYL PHOSPHATE
3091	TOLUENE	404		-0.70	0.94 A	C8H19O4P1	DIBUTYL PHOSPHATE
3092	NITROBENZENE	50		-0.14		C8H19O4P1	DIBUTYL PHOSPHATE
3093	CCL4	50		-1.44	0.63 A	C8H19O4P1	DIBUTYL PHOSPHATE
3094	DI-BUTYL ETHER	50		-0.14		C8H19O4P1	DIBUTYL PHOSPHATE
3095	DI-BUTYL ETHER	236	17	1.18		C8H19O4P1	DIBUTYL PHOSPHATE
3096	DI-I-PR. ETHER	50		0.52	1.15	C8H19O4P1	DIBUTYL PHOSPHATE
3097	HEXANE	50		-2.34		C8H19O4P1	DIBUTYL PHOSPHATE
3098	ME-I-BUT.KETONE	50		1.36	1.19	C8H19O4P1	DIBUTYL PHOSPHATE
3099	S-PENTANOLS	274		2.21		C8H19O4P1	DIBUTYL PHOSPHATE
3100	PARAFFINS	50		-1.96		C8H19O4P1	DIBUTYL PHOSPHATE

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3101	PARAFFINS	404		-1.96		C8H19O4P1	DIBUTYL PHOSPHATE
3102	DIETHYL ETHER	236	17	1.62		C8H19O4P1	OCTYL PHOSPHATE
3103	ME-I-BUT.KETONE	236	17	1.45	1.28	C8H19O4P1	OCTYL PHOSPHATE
3104	CHCL3	405	46	-2.52		C8H20CL1N1	TETRAETHYLAMMONIUM CHLORIDE
3105	OCTANOL	297	46	-2.82	-2.82 =	C8H20I1N1	TETRAETHYLAMMONIUM IODIDE
3106	NITROBENZENE	92	46	-1.65		C8H20I1N1	TETRAETHYLAMMONIUM IODIDE
3107	I-BUTANOL	184		-1.14		C8H21N1O5	TETRAETHANOLAMMONIUM HYDROXIDE
3108	OCTANOL	235		2.85	2.85 =	C9H4CL3N1O2S1	N-(TRICHLOROMETHYLTHIO)PHTHALIMIDE/FOLPET/PHALTAN/
3109	OLEYL ALCOHOL	406		3.13	3.70	C9H4CL3N1O2S1	N-TRICLMETHIOPHTHALIMIDE/PHALTAN/
3110	CYCLOHEXANE	379	19	-1.15		C9H4F3N3	2-TRIFLUOROMETHYL-5-CYANO-BENZIMIDAZOLE
3111	CHCL3	407	14	1.58		C9H5CL1I1N1O1	8-QUINOLINOL,5-CHLORO-7-IODO
3112	HEXANE	299		0.58		C9H5CL1N4	CARBONYL CYANIDE,M-CHLORO-PHENYLHYDRAZONE
3113	CYCLOHEXANE	379	19	1.18		C9H5CL2F3N2	2-TRIFLUOROME-4,6-DICL-5-ME-BENZIMIDAZOLE
3114	CYCLOHEXANE	379	19	-0.07		C9H6CL1F3N2	2-TRIFLUOROME-6-CL-5-ME-BENZIMIDAZOLE
3115	OCTANOL	216		2.73	2.73 =	C9H6CL1N1	6-CHLOROQUINOLINE
3116	OCTANOL	268		2.33	2.33 =	C9H6CL1N1	8-CHLOROQUINOLINE
3117	CHCL3	407	14	1.12		C9H6CL1N1O1	8-QUINOLINOL,5-CHLORO
3118	OCTANOL	302		1.56	1.56 =	C9H6CL1N1O3	PHENOXYACETIC ACID,3-CYANO-4-CHLORO
3119	OCTANE	408		2.63		C9H6N1S1	QUINOLINE,5-BROMO,8-MERCAPTO
3120	OCTANOL	216		1.86	1.86 =	C9H6N2O2	5-NITROQUINOLINE
3121	OCTANOL	216		1.84	1.84 =	C9H6N2O2	6-NITROQUINOLINE
3122	OCTANOL	216		1.82	1.82 =	C9H6N2O2	7-NITROQUINOLINE
3123	OCTANOL	216		1.40	1.40 =	C9H6N2O2	8-NITROQUINOLINE
3124	HEXANE	299		0.21		C9H6N4	CARBONYL CYANIDE,PHENYLHYDRAZONE
3125	OCTANOL	218		1.39	1.39 =	C9H6O2	COUMARIN
3126	CYCLOHEXANE	304		0.48		C9H6O2	COUMARIN
3127	OILS	173		1.21	1.42 B	C9H6O2	COUMARIN
3128	OCTANOL	218		0.61	0.61 =	C9H6O2	1,3-INDANDIONE
3129	OCTANOL	409		0.36	0.36 =	C9H6O2	1,3-INDANEDIONE
3130	CYCLOHEXANE	304		-0.12		C9H6O2	1,3-INDANEDIONE
3131	DIETHYL ETHER	3		1.04	1.03 A	C9H6O6	BENZENE,1,3,5-TRICARBOXYLIC ACID
3132	I-BUTANOL	4		1.48	1.57	C9H6O6	BENZENE,1,3,5-TRICARBOXYLIC ACID
3133	CYCLOHEXANE	141		2.46		C9H7CL1N2O4	STYRENE,2-CHLORO,5-NITRO,B-NITRO,B-METHYL
3134	OCTANOL	302		1.07	1.07 =	C9H7CL1O5	PHENOXYACETIC ACID,3-CARBOXY-4-CHLORO
3135	CYCLOHEXANE	141		3.36		C9H7CL2N1O2	STYRENE,3,4-DICHLORO,B-NITRO,B-METHYL
3136	CYCLOHEXANE	141		4.40		C9H7CL2N1O2	STYRENE,2,6-DICHLORO,B-NITRO,B-METHYL
3137	CYCLOHEXANE	141		3.61		C9H7CL2N2O2	STYRENE,2,4-DICHLORO,B-NITRO,B-METHYL
3138	CYCLOHEXANE	379	19	-0.48		C9H7F3N2	2-TRIFLUOROME-5-METHYLBENZIMIDAZOLE
3139	OCTANOL	10		2.62	2.62 =	C9H7F3O2	M-TRIFLUOROMETHYLPHENYLACETIC ACID
3140	OCTANOL	10		2.36	2.36 =	C9H7F3O3	M-TRIFLUOROMETHYLPHENOXYACETIC ACID
3141	CYCLOHEXANONE	302		3.42		C9H7F3O3	M-TRIFLUOROMETHYLPHENOXYACETIC ACID
3142	CYCLOHEXANOL	302		2.72		C9H7F3O3	M-TRIFLUOROMETHYLPHENOXYACETIC ACID
3143	OCTANOL	10		2.86	2.86 =	C9H7F3O3S1	M-TRIFLUOROMETHYLTHIOPHENOXYACETIC ACID
3144	OCTANOL	10		2.48	2.48 =	C9H7F3O4	M-TRIFLUOROMETHOXYPHENOXYACETIC ACID
3145	OCTANOL	10		2.19	2.19 =	C9H7F3O5S1	M-TRIFLUOROMETHYLSULFONYLPHENOXYACETIC ACID
3146	CYCLOHEXANE	141		1.53		C9H7N1	CINNAMONITRILE
3147	OCTANOL	255		2.03	2.03 =	C9H7N1	QUINOLINE
3148	OCTANOL	309		2.06	2.06 =	C9H7N1	QUINOLINE
3149	CYCLOHEXANE	280		1.26		C9H7N1	QUINOLINE
3150	XYLENE	46		1.14	1.81 B	C9H7N1	QUINOLINE
3151	OCTANOL	186		2.08	2.08 =	C9H7N1	I-QUINOLINE
3152	CYCLOHEXANE	280		1.11		C9H7N1	I-QUINOLINE
3153	OCTANOL	65		1.26	1.26 =	C9H7N1O1	2-QUINOLINOL
3154	OCTANOL	410		1.96	1.96 =	C9H7N1O1	8-QUINOLINOL
3155	OCTANOL	349		2.02	2.02 =	C9H7N1O1	8-QUINOLINOL
3156	CHCL3	411		2.60	1.90 B	C9H7N1O1	8-QUINOLINOL
3157	CHCL3	412		2.64	2.06 B	C9H7N1O1	8-QUINOLINOL
3158	N-BUTANOL	410		1.67	1.81	C9H7N1O1	8-QUINOLINOL
3159	TOLUENE	410		2.21	2.26 B	C9H7N1O1	8-QUINOLINOL
3160	PRIM. PENTANOLS	410		1.79	1.96	C9H7N1O1	8-QUINOLINOL
3161	I-PENT. ACETATE	410		2.24	2.14	C9H7N1O1	8-QUINOLINOL
3162	CCL4	412		2.06	1.89 B	C9H7N1O1	8-QUINOLINOL
3163	ME-I-BUT.KETONE	410		2.13	1.90	C9H7N1O1	8-QUINOLINOL
3164	O-DICL. BENZENE	410		2.48		C9H7N1O1	8-QUINOLINOL
3165	OCTANOL	10		1.18	1.18 =	C9H7N1O2	M-CYANOPHENYLPHENYLACETIC ACID
3166	CYCLOHEXANE	304		0.67		C9H7N1O2	PHTHALIMIDE,N-METHYL
3167	OCTANOL	10		0.93	0.93 =	C9H7N1O3	PHENOXYACETIC ACID,4-CYANO
3168	OCTANOL	10		0.95	0.95 =	C9H7N1O3	PHENOXYACETIC ACID,3-CYANO
3169	CYCLOHEXANE	141		1.41		C9H7N1O4	STYRENE,3,4-DIOXYMETHYLENE,B-NITRO
3170	CHCL3	413		2.51	1.94 B	C9H7N1S1	8-QUINOLINETHIOL
3171	BENZENE	413		2.20	2.08 B	C9H7N1S1	8-QUINOLINETHIOL
3172	CCL4	413		1.91	1.76 B	C9H7N1S1	8-QUINOLINETHIOL
3173	OCTANE	413		1.02		C9H7N1S1	8-QUINOLINETHIOL
3174	OCTANOL	283		2.92	2.92 =	C9H8	INDENE
3175	CYCLOHEXANE	141		3.01		C9H8BR1N1O2	STYRENE,2-BROMO,B-NITRO,B-METHYL
3176	CYCLOHEXANE	141		3.05		C9H8BR1N1O2	STYRENE,3-BROMO,B-NITRO,B-METHYL
3177	CYCLOHEXANE	141		2.63		C9H8CL1N1O2	STYRENE,3-CHLORO,B-NITRO,B-METHYL
3178	CYCLOHEXANE	141		2.97		C9H8CL1N1O2	STYRENE,4-CHLORO,B-NITRO,B-METHYL
3179	CYCLOHEXANE	141		3.31		C9H8CL1N1O2	STYRENE,2-CHLORO,B-NITRO,B-METHYL
3180	OCTANOL	235		2.35	2.35 =	C9H8CL3N1O2S1	CAPTAN
3181	OLEYL ALCOHOL	406		2.15	2.72	C9H8CL3N1O2S1	N-(TRICLMETHIO)-TETRAHYDROPHTHALIMIDE/CAPTAN/
3182	OLEYL ALCOHOL	406		1.65	2.22	C9H8CL3N1O3S1	N-TRICHLMETHIO-3,6-ENDOXOHEXAHYDROPHTHALIMIDE
3183	OLEYL ALCOHOL	406		0.85	1.42	C9H8CL3N1O3S1	N-TRICLMETHIO-4,5-EPOXYHEXAHYDROPHTHALIMIDE
3184	CYCLOHEXANE	141		2.47		C9H8F1N1O2	STYRENE,4-FLUORO,B-NITRO,B-METHYL
3185	CYCLOHEXANE	141		2.57		C9H8F1N1O2	STYRENE,3-FLUORO,B-NITRO,B-METHYL
3186	CYCLOHEXANE	141		2.67		C9H8F1N1O2	STYRENE,2-FLUORO,B-NITRO,B-METHYL
3187	OCTANOL	384		2.37	2.37 =	C9H8F3N1O2	N-METHYL-3-TRIFLUOROMETHYLPHENYLCARBAMATE
3188	OILS	382	24	3.99	4.82 A	C9H8I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,ETHYL ESTER
3189	OILS	382	24	2.30	3.28 A	C9H8I2O4	BENZOIC ACID,3,5-DI-IODO,4-OH,B-HYDROXYETHYL ESTER
3190	OCTANOL	216		1.16	1.16 =	C9H8N2	5-AMINOQUINOLINE
3191	OCTANOL	216		1.79	1.79 =	C9H8N2	8-AMINOQUINOLINE
3192	HEXADECANE	314		-1.78		C9H8N2	O-PHENYLENEDIAMINE
3193	DECANE	314		-1.78		C9H8N2	O-PHENYLENEDIAMINE
3194	CYCLOHEXANE	280		1.28		C9H8N2	QUINOLINE,3-AMINO
3195	OCTANOL	384		1.11	1.11 =	C9H8N2O2	N-METHYL-2-CYANOPHENYLCARBAMATE
3196	OCTANOL	384		0.97	0.97 =	C9H8N2O2	N-METHYL-3-CYANOPHENYLCARBAMATE
3197	OCTANOL	384		0.95	0.95 =	C9H8N2O2	N-METHYL-4-CYANOPHENYLCARBAMATE
3198	OCTANOL	216		0.36	0.36 =	C9H8N2O2S1	8-SULFONAMIDOQUINOLINE
3199	CYCLOHEXANE	141		1.52		C9H8N2O4	STYRENE,2-NITRO,B-NITRO,B-METHYL
3200	CYCLOHEXANE	141		1.59		C9H8N2O4	STYRENE,4-NITRO,B-NITRO,B-METHYL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3201	CYCLOHEXANE	141		1.62		C9H8N2O4	STYRENE,3-NITRO,B-NITRO,B-METHYL
3202	OCTANOL	238		1.88	1.88 =	C9H8O1	ACRYLOPHENONE
3203	CYCLOHEXANE	304		0.96		C9H8O1	1-INDANONE
3204	OCTANOL	218		2.13	2.13 =	C9H8O2	CINNAMIC ACID/TRANS/
3205	CHCL3	149		1.20	2.31 A	C9H8O2	CINNAMIC ACID/TRANS
3206	CHCL3	29	12	1.97	3.01 A	C9H8O2	CINNAMIC ACID/TRANS/
3207	XYLENE	46		0.15	1.97 A	C9H8O2	CINNAMIC ACID/TRANS/
3208	TOLUENE	29	12	1.60	2.98 A	C9H8O2	CINNAMIC ACID/TRANS/
3209	ME-I-BUT.KETONE	149		2.33	2.08	C9H8O2	CINNAMIC ACID/TRANS/
3210	OCTANOL	268		3.25	3.25 =	C9H8O2S1	5,7-DIMETHYL-2-OXO-1,3-BENZOXATHIOL
3211	OCTANOL	186		1.23	1.23 =	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3212	OCTANOL	218		1.19	1.19 =	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3213	DIETHYL ETHER	46		1.15	1.13 A	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3214	CHCL3	29		0.26	1.45 A	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3215	CHCL3	254		0.30	1.46 A	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3216	XYLENE	46		-0.57	1.16 A	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3217	TOLUENE	29		-0.49	1.12 A	C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3218	N-HEPTANE	254		-1.52		C9H8O4	ACETYLSALICYLIC ACID/ASPIRIN/
3219	OCTANOL	10		1.14	1.14 =	C9H8O4	M-CARBOXYPHENYLACETIC ACID
3220	DIETHYL ETHER	414		0.40	0.46 A	C9H8O4	HOMOPHTHALIC ACID
3221	OCTANOL	10		1.83	1.83 =	C9H8O4	ISOPHTHALIC ACID,METHYL ESTER
3222	OCTANOL	10		1.11	1.11 =	C9H8O5	PHENOXYACETIC ACID,M-CARBOXY
3223	CYCLOHEXANOL	302		1.75		C9H8O5	PHENOXYACETIC ACID,M-CARBOXY
3224	OCTANOL	255		1.72	1.72 =	C9H9N1	BENZYLACETONITRILE
3225	OCTANOL	302		1.66	1.66 =	C9H9N1	BENZYLACETONITRILE
3226	OCTANOL	309		2.60	2.60 =	C9H9N1	INDOLE, 3-METHYL
3227	OCTANOL	309		2.68	2.68 =	C9H9N1	INDOLE, 5-METHYL
3228	CYCLOHEXANE	304		-2.21		C9H9N1O1	CINNAMAMIDE
3229	OCTANOL	141		2.52	2.52 =	C9H9N1O2	STYRENE,B-METHYL-B-NITRO
3230	CYCLOHEXANE	141		2.69		C9H9N1O2	STYRENE,B-METHYL-B-NITRO
3231	OCTANOL	141	26	2.28	2.28 =	C9H9N1O2	STYRENE,4-METHYL-B-NITRO
3232	CYCLOHEXANE	141		2.40		C9H9N1O2	STYRENE,2-METHYL,B-NITRO
3233	CYCLOHEXANE	141		2.42		C9H9N1O2	STYRENE,4-METHYL,B-NITRO
3234	OCTANOL	56		1.88	1.88 =	C9H9N1O3	O-AMINOBENZOIC ACID,N-ACETYL
3235	DIETHYL ETHER	3		-0.41	-0.25 A	C9H9N1O3	GLYCINE,N-BENZOYL/HIPPURIC ACID/
3236	DIETHYL ETHER	46		-0.22	-0.07 A	C9H9N1O3	GLYCINE,N-BENZOYL /HIPPURIC ACID/
3237	OCTANOL	141		2.30	2.30 =	C9H9N1O3	STYRENE,3-METHOXY-B-NITRO
3238	CYCLOHEXANE	141		1.73		C9H9N1O3	STYRENE,4-METHOXY,B-NITRO
3239	CYCLOHEXANE	141		1.89		C9H9N1O3	STYRENE,3-METHOXY,B-NITRO
3240	CYCLOHEXANE	141		2.15		C9H9N1O3	STYRENE,2-METHOXY,B-NITRO
3241	OCTANOL	141		1.88	1.88 =	C9H9N1O4	STYRENE,4-HYDROXY-3-METHOXY-B-NITRO
3242	CYCLOHEXANE	141		0.04		C9H9N1O4	STYRENE,4-HYDROXY,3-METHOXY,B-NITRO
3243	OCTANOL	393	63	0.35	0.35 =	C9H9N3O2S2	SULFATHIAZOLE
3244	OCTANOL	56		0.05	0.05 =	C9H9N3O2S2	SULFATHIAZOLE
3245	DIETHYL ETHER	342		-0.72	0.21 B	C9H9N3O2S2	SULFATHIAZOLE
3246	DIETHYL ETHER	113	15	-0.99	-0.03 B	C9H9N3O2S2	SULFATHIAZOLE
3247	CHCL3	343	2	-0.82	-0.16 N	C9H9N3O2S2	SULFATHIAZOLE
3248	CHCL3	113	15	-0.75	-0.09 N	C9H9N3O2S2	SULFATHIAZOLE
3249	CHCL3	326		-0.87	-0.21 N	C9H9N3O2S2	SULFATHIAZOLE
3250	CHCL3	344	44	-0.80	-0.14 N	C9H9N3O2S2	SULFATHIAZOLE
3251	CHCL3	393	63	-0.73	-0.68 N	C9H9N3O2S2	SULFATHIAZOLE
3252	CHCL3	415	44	-0.74	-0.08 N	C9H9N3O2S2	SULFATHIAZOLE
3253	BENZENE	343	2	-0.96	0.43 A	C9H9N3O2S2	SULFATHIAZOLE
3254	1-PENT. ACETATE	343	2	-0.28	-0.47	C9H9N3O2S2	SULFATHIAZOLE
3255	CCL4	343	2	-1.57	0.54 A	C9H9N3O2S2	SULFATHIAZOLE
3256	N-HEPTANE	415	44	-4.60		C9H9N3O2S2	SULFATHIAZOLE
3257	OCTANOL	235		3.23	3.23 =	C9H10	ALLYLBENZENE
3258	OCTANOL	9		3.35	3.35 =	C9H10	1-PROPENE,1-PHENYL
3259	HEXANE	391		0.58		C9H10CL1N1O2	N-METHYL CARBAMATE,3-METHYL,4-CHLOROPHENYL
3260	OCTANOL	384		2.57	2.57 =	C9H10CL1N1O2	N-METHYL-3-METHYL-4-CHLOROPHENYLCARBAMATE
3261	N-HEPTANE	416	14	0.49		C9H10CL1N1O3	P-AMINOSALICYLIC ACID,2-CHLOROETHYL ESTER
3262	OLEYL ALCOHOL	406		2.40	2.97	C9H10CL3N1O2S1	N-TRICLMETHIOHEXAHYDROPHTHALIMIDE
3263	CHCL3	306		0.48	1.60 A	C9H10I1N1O4S1	N-(P-IODOBENZENESULFONYL)ALANINE
3264	CCL4	306	12	-1.40	0.65 A	C9H10I1N1O4S1	N-(P-IODOBENZENESULFONYL)ALANINE
3265	CLCH2CH2CL	306		0.74		C9H10I1N1O4S1	N-(P-IODOBENZENESULFONYL)ALANINE
3266	DIETHYL ETHER	306		0.62	0.70 A	C9H10I1N1O5S1	N-(P-IODOBENZENESULFONYL)SERINE
3267	CHCL3	306	12	-1.30	0.04 A	C9H10I1N1O5S1	N-(P-IODOBENZENESULFONYL)SERINE
3268	ETHYL ACETATE	306		1.34	1.49 A	C9H10I1N1O5S1	N-(P-IODOBENZENESULFONYL)SERINE
3269	CLCH2CH2CL	306		-0.82		C9H10I1N1O5S1	N-(P-IODOBENZENESULFONYL)SERINE
3270	OCTANOL	206		2.35	2.35 =	C9H10N2	BENZIMIDAZOLE,5,6-DIMETHYL
3271	OCTANOL	10		0.26	0.26 =	C9H10N2O4	PHENOXYACETIC ACID,3-UREIDO
3272	OCTANOL	56		0.54	0.54 =	C9H10N4O2S2	SULFAMETHIZOLE
3273	CHCL3	343	2	-0.05	0.53 N	C9H10N4O2S2	SULFAMETHIZOLE
3274	CHCL3	415	44	-0.43	0.21 N	C9H10N4O2S2	SULFAMETHIZOLE
3275	BENZENE	343	2	-1.77	-0.36 A	C9H10N4O2S2	SULFAMETHIZOLE
3276	1-PENT. ACETATE	343	2	0.34	0.18	C9H10N4O2S2	SULFAMETHIZOLE
3277	CCL4	343	2	-1.82	0.33 A	C9H10N4O2S2	SULFAMETHIZOLE
3278	N-HEPTANE	415	44	-3.83		C9H10N4O2S2	SULFAMETHIZOLE
3279	OCTANOL	218		2.94	2.94 =	C9H10O1	ALLYLPHENYL ETHER
3280	OCTANOL	56		1.95	1.95 =	C9H10O1	CINNAMYL ALCOHOL
3281	CYCLOHEXANE	325		0.61		C9H10O1	4-INDANOL
3282	CYCLOHEXANE	325		0.48		C9H10O1	5-INDANOL
3283	OCTANOL	255		1.44	1.44 =	C9H10O1	2-PROPANONE,1-PHENYL
3284	OCTANOL	255		1.96	1.96 =	C9H10O2	ACETIC ACID,BENZYL ESTER
3285	CHCL3	254		0.71	1.83 A	C9H10O2	P-HYDROXYPROPIOPHENONE
3286	N-HEPTANE	254		-0.92		C9H10O2	P-HYDROXYPROPIOPHENONE
3287	OCTANOL	10		1.95	1.95 =	C9H10O2	M-METHYLPHENYLACETIC ACID
3288	OCTANOL	10		1.86	1.86 =	C9H10O2	P-METHYLPHENYLACETIC ACID
3289	OCTANOL	255		1.83	1.83 =	C9H10O2	PHENYLACETIC ACID,METHYL ESTER
3290	OILS	362		0.51	1.68 A	C9H10O2	A-PHENYLPROPIONIC ACID
3291	OILS	385		0.75	1.91 A	C9H10O2	A-PHENYLPROPIONIC ACID
3292	OCTANOL	255		1.84	1.84 =	C9H10O2	B-PHENYLPROPIONIC ACID
3293	CHCL3	46		1.10	2.22 A	C9H10O2	B-PHENYLPROPIONIC ACID
3294	OILS	361		0.72	1.91 A	C9H10O2	B-PHENYLPROPIONIC ACID
3295	OILS	417		0.82	1.92 A	C9H10O2	B-PHENYLPROPIONIC ACID
3296	XYLENE	46		0.46	2.29 A	C9H10O2	B-PHENYLPROPIONIC ACID
3297	DIETHYL ETHER	248		1.34	1.29 A	C9H10O3	BENZALDEHYDE,3-ETHOXY-4-HYDROXY/ETHYL VANILLIN/
3298	CYCLOHEXANE	248		0.03		C9H10O3	BENZALDEHYDE,3-ETHOXY-4-HYDROXY/ETHYL VANILLIN/
3299	BENZENE	248		1.43	2.81 A	C9H10O3	BENZALDEHYDE,3-ETHOXY-4-HYDROXY/ETHYL VANILLIN/
3300	CLCH2CH2CL	248		1.86		C9H10O3	BENZALDEHYDE,3-ETHOXY-4-HYDROXY/ETHYL VANILLIN/

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3301	OCTANOL	56		2.47	2.47 =	C9H1003	P-HYDROXYBENZOIC ACID,ETHYL ESTER
3302	OCTANOL	10		1.50	1.50 =	C9H1003	M-METHOXYPHENYLACETIC ACID
3303	OCTANOL	10		1.42	1.42 =	C9H1003	P-METHOXYPHENYLACETIC ACID
3304	OILS	383		0.45	1.63 A	C9H1003	P-METHOXYPHENYLACETIC ACID
3305	OCTANOL	10		1.78	1.78 =	C9H1003	M-METHYLPHENOXYACETIC ACID
3306	OCTANOL	10		2.10	2.10 =	C9H1003	O-METHYLPHENOXYACETIC ACID
3307	OCTANOL	268	19	1.86	1.86 =	C9H1003	P-METHYLPHENOXYACETIC ACID
3308	CYCLOHEXANONE	302		2.46	2.46 =	C9H1003	P-METHYLPHENOXYACETIC ACID
3309	CYCLOHEXANOL	302		2.05	2.05 =	C9H1003	P-METHYLPHENOXYACETIC ACID
3310	OCTANOL	10		1.90	1.90 =	C9H1003S1	PHENOXYACETIC ACID,3-METHYLTHIO
3311	OILS	173		0.86	1.98 A	C9H1004	GLYCOL SALICYLATE
3312	OCTANOL	10		0.93	0.93 =	C9H1004	PHENOXYACETIC ACID,2-METHOXY
3313	OCTANOL	10		1.23	1.23 =	C9H1004	PHENOXYACETIC ACID,4-METHOXY
3314	OCTANOL	10		1.38	1.38 =	C9H1004	PHENOXYACETIC ACID,3-METHOXY
3315	CYCLOHEXANONE	302		2.40		C9H1004	PHENOXYACETIC ACID,3-METHOXY
3316	CYCLOHEXANOL	302		1.80		C9H1004	PHENOXYACETIC ACID,3-METHOXY
3317	OCTANOL	10		0.06	0.06 =	C9H1004S1	M-METHYLSULFONYLPHENYLACETIC ACID
3318	DIETHYL ETHER	323		1.07	1.05 A	C9H1005	BENZOIC ACID,4-HYDROXY,3,5-DIMETHOXY (ME-SYRINGATE)
3319	OCTANOL	10		0.01	0.01 =	C9H1005S1	PHENOXYACETIC ACID,M-METHYLSULFONYL
3320	CYCLOHEXANOL	302		0.88		C9H1005S1	PHENOXYACETIC ACID,M-METHYLSULFONYL
3321	OCTANOL	255		3.72	3.72 =	C9H11BR1	PROPYLBROMIDE,G-PHENYL
3322	OCTANOL	255		3.55	3.55 =	C9H11CL1	PROPYLCHLORIDE,G-PHENYL
3323	HEXANE	391		1.41		C9H11CL3N1O3P1	ETHYLPHOSPHORAMIDATE,O-ME,O-(2,4,5-TRICLPHENYL)
3324	OCTANOL	255		2.95	2.95 =	C9H11F1	PROPYLFLUORIDE,G-PHENYL
3325	OCTANOL	226		-1.38	-1.38 =	C9H11F1N2O5	2'-DEOXY-5-FLUOROURIDINE (27640)
3326	OCTANOL	56		3.90	3.90 =	C9H11I1	PROPYLIODIDE,G-PHENYL
3327	BENZENE	72		0.18	1.55 A	C9H11N1O1	O-ACETAMIDOTOLUENE
3328	OCTANOL	255		0.91	0.91 =	C9H11N1O1	PROPIONAMIDE,3-PHENYL
3329	OILS	173		-0.20	1.01 A	C9H11N1O2	ACETANILIDE,P-METHOXY/METHACETIN/
3330	OILS	224		0.30	1.47 A	C9H11N1O2	ACETANILIDE,P-METHOXY/METHACETIN/
3331	OCTANOL	349		2.57	2.57 =	C9H11N1O2	O-AMINOBENZOIC ACID,ETHYL ESTER
3332	1-PENT. ACETATE	418	3	2.50	2.41	C9H11N1O2	P-AMINOBENZOIC ACID,ETHYL ESTER
3333	OLEYL ALCOHOL	390	44	1.61	2.15	C9H11N1O2	P-AMINOBENZOIC ACID,ETHYL ESTER
3334	OCTANOL	186		2.30	2.30 =	C9H11N1O2	ETHYLCARBAMATE,N-PHENYL
3335	OILS	173		1.99	3.00 A	C9H11N1O2	ETHYLCARBAMATE,N-PHENYL
3336	OILS	224		2.18	3.26 A	C9H11N1O2	ETHYLCARBAMATE,N-PHENYL
3337	OCTANOL	276		0.98	0.98 =	C9H11N1O2	O-METHOXYACETANILIDE
3338	OCTANOL	276		1.14	1.14 =	C9H11N1O2	P-METHOXYACETANILIDE
3339	HEXANE	391		0.04		C9H11N1O2	N-METHYL CARBAMATE,3-METHYLPHENYL
3340	OCTANOL	384		1.70	1.70 =	C9H11N1O2	N-METHYL-M-TOLYLCARBAMATE
3341	OCTANOL	384		1.46	1.46 =	C9H11N1O2	N-METHYL-O-TOLYLCARBAMATE
3342	OCTANOL	384		1.66	1.66 =	C9H11N1O2	N-METHYL-P-TOLYLCARBAMATE
3343	OCTANOL	56		-1.43	-1.43 =	C9H11N1O2	PHENYLALANINE, DL
3344	OCTANOL	384		1.92	1.92 =	C9H11N1O2S1	N-METHYL-4-METHYLTHIOPHENYLCARBAMATE
3345	N-HEPTANE	370	14	0.98		C9H11N1O3	P-AMINOSALICYLIC ACID,ETHYL ESTER
3346	OCTANOL	384		0.81	0.81 =	C9H11N1O3	N-METHYL-2-METHOXYPHENYLCARBAMATE
3347	OCTANOL	384		1.30	1.30 =	C9H11N1O3	N-METHYL-3-METHOXYPHENYLCARBAMATE
3348	OCTANOL	384		1.20	1.20 =	C9H11N1O3	N-METHYL-4-METHOXYPHENYLCARBAMATE
3349	OCTANOL	56		-2.26	-2.26 =	C9H11N1O3	TYROSINE, L
3350	N-HEPTANE	370	14	-0.82		C9H11N1O4	P-AMINOSALICYLIC ACID,2-HYDROXYETHYL ESTER
3351	OCTANOL	56		3.66	3.66 =	C9H12	ISOPROPYLBENZENE
3352	OCTANOL	298		3.66	3.66 =	C9H12	ISOPROPYLBENZENE
3353	OCTANOL	255		3.68	3.68 =	C9H12	PROPYLBENZENE
3354	OCTANOL	218		3.57	3.57 =	C9H12	PROPYLBENZENE
3355	BENZENE	311	6	-1.15		C9H12B1N1O4	PHENYLBORONIC ACID,M-ETHOXYACETAMIDO
3356	BENZENE	311	6	-2.41		C9H12B1N1O4	PHENYLBORONIC ACID,P-B-ALANINYL
3357	CHCL3	396	31	2.31	1.75 B	C9H12CL1N1	4-CHLOROAMPHETAMINE
3358	N-HEPTANE	396	31	0.96		C9H12CL1N1	4-CHLOROAMPHETAMINE
3359	N-BUTANOL	295	52	0.00	-0.51	C9H12CL1N1O2	PHENYLALANINE HYDROCHLORIDE
3360	N-BUTANOL	295	52	-0.25	-0.86	C9H12CL1N1O3	TRYROSINE HYDROCHLORIDE
3361	OCTANOL	341	60	0.17	0.17 =	C9H12N2	NORNICOTINE
3362	OCTANOL	186	27	0.98		C9H12N2O1	UREA,1,1-DIMETHYL-3-PHENYL
3363	OCTANOL	218		1.02	1.02 =	C9H12N2O1	UREA,1,3-DIMETHYL PHENYL
3364	N-HEPTANE	419		-2.52		C9H12N2O1	UREA,ETHYLPHENYL-
3365	N-HEPTANE	419		-2.16		C9H12N2O1	UREA,METHYL,M-TOLYL-
3366	N-HEPTANE	419		-1.85		C9H12N2O1	UREA,METHYL,O-TOLYL-
3367	N-HEPTANE	419		-1.89		C9H12N2O1	UREA,METHYL,P-TOLYL-
3368	CHCL3	399	1	2.49	2.97 N	C9H12N2O2S1	BARBITURIC ACID,5-ALLYL,5-ETHYL,2-THIO
3369	I-PENT. ACETATE	399	1	2.92	2.85	C9H12N2O2S1	BARBITURIC ACID,5-ALLYL,5-ETHYL,2-THIO
3370	CCL4	399	1	1.36	3.02 A	C9H12N2O2S1	BARBITURIC ACID,5-ALLYL,5-ETHYL,2-THIO
3371	OCTANOL	399		0.95	0.95 =	C9H12N2O3	BARBITURIC ACID,5-ALLYL,5-ETHYL
3372	CHCL3	399	1	0.12	0.69 N	C9H12N2O3	BARBITURIC ACID,5-ALLYL,5-ETHYL
3373	BENZENE	399	1	-0.51	0.87 A	C9H12N2O3	BARBITURIC ACID,5-ALLYL-5-ETHYL
3374	I-PENT. ACETATE	399	1	0.98	0.84	C9H12N2O3	BARBITURIC ACID,5-ALLYL,5-ETHYL
3375	CCL4	399	1	-1.20	0.84 A	C9H12N2O3	BARBITURIC ACID,5-ALLYL,5-ETHYL
3376	N-BUTANOL	420	37	-0.80	-1.62	C9H12N2O6	URIDINE
3377	N-BUTANOL	253	36	-0.92	-1.79	C9H12N2O6	URIDINE
3378	CCL4	234	12	0.74		C9H12N4O3	8-METHOXYCAFFEINE
3379	CYCLOHEXANE	132		0.89		C9H12O1	PHENOL,5-ETHYL,3-METHYL
3380	CYCLOHEXANE	325		0.73		C9H12O1	PHENOL,5-ETHYL,3-METHYL
3381	CYCLOHEXANE	325		0.74		C9H12O1	PHENOL,3-ETHYL,4-METHYL
3382	CYCLOHEXANE	325		0.97		C9H12O1	PHENOL,3-ETHYL,2-METHYL
3383	CYCLOHEXANE	325		1.01		C9H12O1	PHENOL,4-ETHYL,2-METHYL
3384	CYCLOHEXANE	325		1.02		C9H12O1	PHENOL,5-ETHYL,2-METHYL
3385	CYCLOHEXANE	325		1.06		C9H12O1	PHENOL,2-ETHYL,5-METHYL
3386	OCTANOL	255		1.88	1.88 =	C9H12O1	PROPANOL,3-PHENYL
3387	HEXANE	372		0.08		C9H12O1	PROPANOL,3-PHENYL
3388	CYCLOHEXANE	325		0.83		C9H12O1	M-PROPYLPHENOL
3389	CYCLOHEXANE	325		1.18		C9H12O1	O-PROPYLPHENOL
3390	CYCLOHEXANE	133		1.08		C9H12O1	O-I-PROPYLPHENOL
3391	CYCLOHEXANE	325		0.86		C9H12O1	P-PROPYLPHENOL
3392	CYCLOHEXANE	325		0.77		C9H12O1	P-I-PROPYLPHENOL
3393	CYCLOHEXANE	133		0.81		C9H12O1	P-I-PROPYLPHENOL
3394	CYCLOHEXANE	325		0.97		C9H12O1	2,3,5-TRIMETHYLPHENOL
3395	CYCLOHEXANE	325		0.94		C9H12O1	2,4,5-TRIMETHYLPHENOL
3396	CYCLOHEXANE	325		1.24		C9H12O1	2,4,6-TRIMETHYLPHENOL
3397	CYCLOHEXANE	325		0.63		C9H12O1	3,4,5-TRIMETHYLPHENOL
3398	DIETHYL ETHER	332		2.37	2.29 A	C9H12O2	BENZENE,1,2-DIHYDROXY-4-PROPYL
3399	DI-BUTYL ETHER	332		1.65		C9H12O2	BENZENE,1,2-DIHYDROXY,4-PROPYL
3400	DI-I-PR. ETHER	332		2.03	2.94	C9H12O2	BENZENE,1,2-DIHYDROXY,4-PROPYL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3401	OIETHYL ETHER	323		-1.17	-0.91 A	C9H12O2	OIMETHYLGUAIACOL
3402	OILS	327		1.78	2.80 A	C9H12O2	PHENOL,2-METHOXY-4-ETHYL/P-ETHYLGUAIACOL//
3403	PARAFFINS	327		1.20		C9H12O2	PHENOL,2-METHOXY-4-ETHYL/P-ETHYLGUAIACOL/
3404	OCTANOL	238		1.53	1.53 =	C9H12O3	BENZENE,1,2,3-TRIMETHOXY
3405	OILS	327		1.04	2.13 A	C9H12O3	PHENOL,2,6-OIMETHOXY-4-METHYL
3406	PARAFFINS	327		0.15		C9H12O3	PHENOL,2,6-OIMETHOXY-4-METHYL
3407	OCTANOL	238		0.70	0.70 =	C9H12O3	PHENYLGLYCEROL
3408	OIETHYL ETHER	323		-0.45	-0.28 A	C9H12O4	BENZYLALCOHOL,3,5-OIMETHOXY-4-HYOROXY/SYRINGYL ALCOHOL/
3409	BENZENE	311	6	0.35		C9H13BO2	PHENYLBORONIC ACIO,2,4,6-TRIMETHYL
3410	OCTANOL	373		-1.43	-1.43 =	C9H13CL1N2O1	N1-PROPYLNICOTINAMIOE CHLORIOE
3411	CHCL3	396	31	2.17	1.63 B	C9H13N1	AMPHETAMINE
3412	N-HEPTANE	138		0.53		C9H13N1	AMPHETAMINE
3413	N-HEPTANE	396	31	0.28		C9H13N1	AMPHETAMINE
3414	N-HEPTANE	421	44	1.57		C9H13N1	BENZYLOIMETHYLAMINE
3415	OIETHYL ETHER	46		1.08	1.82 B	C9H13N1	BENZYLETHYLAMINE
3416	DIETHYL ETHER	374		1.21	1.92 B	C9H13N1	BENZYLETHYLAMINE
3417	XYLENE	46		1.72	2.37 B	C9H13N1	BENZYLETHYLAMINE
3418	XYLENE	422		0.96	1.60 B	C9H13N1	ETHYL AMINE,1-METHYL,2-PHENYL
3419	OIETHYL ETHER	374		1.08	1.80 B	C9H13N1	PHENYL-I-PROPYLAMINE
3420	OCTANOL	255		1.83	1.83 =	C9H13N1	PROPYLAMINE,3-PHENYL
3421	OCTANOL	312		2.45	2.45 =	C9H13N1	N-PROPYLANILINE
3422	CYCLOHEXANE	337		2.95		C9H13N1	O-TOLUIOINE,N,N-OIMETHYL
3423	CHCL3	396	31	-1.45	-1.46 B	C9H13N1O1	NOREPHEORINE
3424	N-HEPTANE	396	31	-3.00		C9H13N1O1	NOREPHEORINE
3425	CHCL3	396	31	-1.00	-1.07 B	C9H13N1O1	NORPSEUOOEPHEORINE
3426	N-HEPTANE	396	31	-2.00		C9H13N1O1	NORPSEUOOEPHEORINE
3427	HEXANE	376		1.53		C9H13N1O4	N-ME-N-ACETYLCARBAMIC ACIO,2,3-OI-H-2-MEFURANYL ESTER
3428	OCTANOL	283	65	0.37	0.37 =	C9H13N3O1.H3PO4	IPRONIAZIO PHOSPHATE
3429	OCTANOL	227		-2.13	-2.13 =	C9H13N3O5	I-B-O-ARABINOFURANOSYLCYTOSINE HCL(63878)(PKA=4.21)
3430	N-BUTANOL	420	37	-0.97	-1.86	C9H13N3O5	CYTIOINE
3431	OCTANOL	227		-0.79	-0.79 =	C9H13N3O5	CYTOSINE ARABINOSIOE (63878)
3432	OCTANOL	397		1.25	1.25 =	C9H13N5	AOENINE,9-BUTYL
3433	OCTANOL	397		0.14	0.14 =	C9H13N5O1	AOENINE,9-(1-HYOROXYMETHYL-PROPYL)
3434	OCTANOL	65	53	-2.69	-2.69 =	C9H14BR1N1	BUTYLPYRIOINIUM BROMIOE
3435	OCTANOL	65	46	-2.07	-2.07 =	C9H14BR1N1	PHENYLTRIMETHYLAMMONIUM BROMIOE
3436	OCTANOL	268	46	-1.09	-1.09 =	C9H14CL1N1	3-PHENYLPROPYLAMINE HYOROCHLORIOE
3437	OCTANOL	341	60	0.82	0.82 =	C9H14N2	N,N-OIMETHYL-2-(3-PYRIOYL)ETHYLAMINE
3438	OCTANOL	341	60	0.54	0.54 =	C9H14N2	N-ETHYL-2-(3-PYRIOYL)ETHYLAMINE
3439	OCTANOL	341	60	0.90	0.90 =	C9H14N2	N-PROPYL-3-(3-PYRIOYL)METHYLAMINE
3440	OCTANOL	341	60	0.82	0.82 =	C9H14N2	N-I-PROPYL-3-PYRIOYLMETHYLAMINE
3441	CHCL3	399	1	1.54	1.09 B	C9H14N2O3	BARBITURIC ACIO,5,5-OIETHYL,I-METHYL/METHARBITAL/
3442	1-PENT. ACETATE	399	1	1.31	1.18	C9H14N2O3	BARBITURIC ACIO,5,5-OIETHYL,1-METHYL/METHARBITAL/
3443	CCL4	399	1	0.31	0.23 B	C9H14N2O3	BARBITURIC ACIO,5,5-OIETHYL,1-METHYL/METHARBITAL/
3444	OCTANOL	399		0.97	0.97 =	C9H14N2O3	BARBITURIC ACIO,5-ETHYL-5-I-PROPYL/PROBARBITAL/
3445	CHCL3	399	1	0.20	0.77 N	C9H14N2O3	BARBITURIC ACIO,5-ETHYL-5-I-PROPYL/PROBARBITAL/
3446	OILS	345		-0.14	1.07 A	C9H14N2O3	BARBITURIC ACIO,5-ETHYL-5-I-PROPYL/PROBARBITAL/
3447	BENZENE	399	1	-0.58	0.80 A	C9H14N2O3	BARBITURIC ACIO,5-ETHYL-5-I-PROPYL/PROBARBITAL/
3448	1-PENT. ACETATE	399	1	0.95	0.81	C9H14N2O3	BARBITURIC ACIO,5-ETHYL-5-I-PROPYL/PROBARBITAL/
3449	CCL4	399	1	-1.21	-0.85 N	C9H14N2O3	BARBITURIC ACIO,5-ETHYL-5-I-PROPYL/PROBARBITAL/
3450	OCTANOL	181	10	0.40	0.40 =	C9H14N3O8P1	CYTIOYLIC ACIO
3451	N-BUTANOL	181	10	-0.15		C9H14N3O8P1	CYTIOYLIC ACIO
3452	PRIM. PENTANOLS	181	10	0.43		C9H14N3O8P1	CYTIOYLIC ACIO
3453	HEXANOL	181	18	-0.15		C9H14N3O8P1	CYTIOYLIC ACIO
3454	OCTANOL	134		0.38	0.38 =	C9H14N4O2S1	6-(2-PENHYOROPYRANYL)-4-AM-3-METHIO-1,2,4-TRIAZINONE
3455	OIETHYL ETHER	423		2.63	2.42 A	C9H14O1S1	A-CYCLOHEXYLTHIOACRYLIC ACIO
3456	OCTANOL	186		3.84	3.84 =	C9H14O1SI1	PHENOL,P-(TRIMETHYLSILYL)
3457	OILS	347		1.94	2.96 A	C9H14O2	SORBIC ACIO,PROPYL ESTER
3458	OIETHYL ETHER	3		0.15	0.25 A	C9H14O6	GLYCERYL TRIACETATE
3459	OILS	2		-0.36	0.14 B	C9H14O6	GLYCERYL TRIACETATE
3460	OILS	214		-0.52	0.01 B	C9H14O6	GLYCERYL TRIACETATE
3461	OIETHYL ETHER	3		-0.37	-0.21 A	C9H14O7	TRIMETHYL CITRATE
3462	OILS	2		-1.33	0.03 A	C9H14O7	TRIMETHYL CITRATE
3463	OCTANOL	298		4.72	4.72 =	C9H14SI1	SILANE, PHENYL-TRIMETHYL
3464	BENZENE	311	6	1.52		C9H15BO2SI1	PHENYLBORONIC ACIO,P-TRIMETHYLSILICYL
3465	OCTANOL	348		0.41	0.41 =	C9H15N1O2	N-BUTYROYLCYCLOBUTANECARBOXAMIOE
3466	OCTANOL	348		0.26	0.26 =	C9H15N1O2	N-I-BUTYROYLCYCLOBUTANECARBOXAMIOE
3467	OCTANOL	227		2.83	2.83 =	C9H16CL1N3O2	1-(2-CLET)-3-CYCLOHEXYL-1-NITROSOUREA(79037)
3468	OECANOL	289		2.69		C9H16CL1N3O2	1-(2-CLET)-3-CYCLOHEXYL-1-NITROSOUREA(79037)
3469	OCTANOL	80		1.40	1.40 =	C9H16N1O3	UREA, 1,3-OIBUTYRYL
3470	OILS	168		-0.23	0.25 B	C9H16N2O2	OIPROPYLHYOANTOIN
3471	OCTANOL	134		1.85	1.85 =	C9H16N4O1S1	3-METHIO-4-AMINO-6-I-PENT-1,2,4-TRIAZINE-5-ONE
3472	OCTANOL	134		2.06	2.06 =	C9H16N4O1S1	3-I-PRTHIO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
3473	OCTANOL	134		2.12	2.12 =	C9H16N4O1S1	3-N-PRTHIO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
3474	OCTANOL	5		1.57	1.57 =	C9H16O4	AZELAIC ACIO
3475	DIETHYL ETHER	212		1.20	1.17 A	C9H16O4	AZELAIC ACID
3476	OIETHYL ETHER	194	12	0.97	1.00 A	C9H16O4	AZELAIC ACIO
3477	CHCL3	194	12	-0.58	0.71 A	C9H16O4	AZELAIC ACIO
3478	1-BUTANOL	4		1.66	1.83	C9H16O4	AZELAIC ACID
3479	OCTANOL	235	67	2.29	2.29 =	C9H17N1	METHYL-I-PROPYL-(I,1-OIMETHYLPROPYN-3-YL)AMINE
3480	OILS	290		0.26	1.43 A	C9H17N1O3	OIETHYL ACETURETHANE/OETONAL/
3481	N-BUTANOL	377		-0.74	-1.56	C9H17N1O4	ACETYLCARNITINE
3482	CHCL3	424	46	-3.76		C9H18I1N1O2	N-METHYL4-ACETYL PIPERIOINE METHIOOIOE
3483	OCTANOL	218		0.70	0.70 =	C9H18N2O4	MEPROBAMATE
3484	PARAFFINS	241		-0.07		C9H18N2S1	N-HEXYLETHYLENETHIOUREA
3485	OCTANOL	226		2.63	2.63 =	C9H18N6	HEXAMETHYLMELAMINE (13875)
3486	CHCL3	425		-1.92	-1.19 N	C9H18O6	GLUCOSE,2,3,6-TRIMETHYL
3487	CHCL3	425		-1.51	-0.80 N	C9H18O6	A-METHYLGLUCOSIOE,2,3-OIMETHYL
3488	OILS	292		0.76	1.87 A	C9H19N1O1	N,N-OIETHYLVALERAMIOE
3489	CHCL3	424	46	-3.05		C9H20I1N1	1,2,6-TRIMETHYLPIPERIDINE METHIOOIOE
3490	CHCL3	424	46	-2.94		C9H20I1N1	1,3,5-TRIMETHYLPIPERIOINE METHIOOIOE
3491	OIETHYL ETHER	3		1.04	1.79 B	C9H20N2O1	TETRAETHYLUREA
3492	OIETHYL ETHER	378	44	-0.92	0.13 B	C9H20N2O2	N,N-OIMETHYLCARBAMIC ACIO,OIETAMINOETHYL ESTER
3493	DIETHYL ETHER	378	44	-1.08	-0.01 B	C9H20N2O2	N-ETHYLCARBAMIC ACID,OIETAMINOETHYL ESTER
3494	OCTANOL	218		2.79	2.79 =	C9H21N1	TRIPROPYLAMINE
3495	TOLUENE	68		2.52	2.47 B	C9H21N1	TRIPROPYLAMINE
3496	OCTANOL	268		-0.88	-0.88 =	C9H21N3.2.H2SO4	OCTYLGUANIDIUM SULFATE
3497	CCL4	426		1.86	2.53 N	C9H21O4P1	TRIPROPYLPHOSPHATE
3498	HEXANE	426		0.88	.	C9H21O4P1	TRIPROPYLPHOSPHATE
3499	OCTANOL	297	46	-1.84	-1.84 =	C9H22I1N1	TRIMETHYL-HEXYL-AMMONIUM IOOIOE
3500	OIETHYL ETHER	3		-0.24	0.65 B	C9H22N2	PENTANE,2-AMINO,5-DIETHYLAMINO

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3501	I-BUTANOL	4		1.08	1.01	C9H22N2	PENTANE,2-AMINO,5-DIETHYLAMINO
3502	OCTANOL	206	27	5.18	5.18 =	C10H3CL2F3N4	QUINOXALINE IMIDAZOLE,2-TRIFLOROME-5,7-DICL
3503	CYCLOHEXANE	141		2.84		C10H4BR2O2	1,4-NAPHTHOQUINONE,2,3-DIBROMO
3504	OCTANOL	206	27	3.91	3.91 =	C10H4CL1F3N4	QUINOXALINE IMIDAZOLE,2-TRIFLOROME,6-CL
3505	CYCLOHEXANE	304		2.28		C10H4CL2N2	MALONONITRILE,3,4-DICHLOROBENZAL
3506	CYCLOHEXANE	304		2.45		C10H4CL2N2	MALONONITRILE,2,6-DICHLOROBENZAL
3507	CYCLOHEXANE	304		2.71		C10H4CL2N2	MALONONITRILE,2,4-DICHLOROBENZAL
3508	CYCLOHEXANE	141		2.56		C10H4CL2O2	1,4-NAPHTHOQUINONE,2,3-DICHLORO
3509	CYCLOHEXANE	304		1.97		C10H5BR1N2	MALONONITRILE,3-BROMOBENZAL
3510	CYCLOHEXANE	304		2.03		C10H5BR1N2	MALONONITRILE,4-BROMOBENZAL
3511	CYCLOHEXANE	304		2.26		C10H5BR1N2	MALONONITRILE,2-BROMOBENZAL
3512	CYCLOHEXANE	141		2.12		C10H5BR1O2	1,4-NAPHTHOQUINONE,2-BROMO
3513	CYCLOHEXANE	304		1.79		C10H5CL1N2	MALONONITRILE,3-CHLOROBENZAL
3514	CYCLOHEXANE	304		1.82		C10H5CL1N2	MALONONITRILE,4-CHLOROBENZAL
3515	CYCLOHEXANE	304		2.10		C10H5CL1N2	MALONONITRILE,2-CHLOROBENZAL
3516	OCTANOL	141		2.15	2.15 =	C10H5CL1O2	1,4-NAPHTHOQUINONE,2-CHLORO
3517	CYCLOHEXANE	141		1.91		C10H5CL1O2	1,4-NAPHTHOQUINONE,2-CHLORO
3518	HEXANE	317		5.05		C10H5CL7	HEPTACHLOR
3519	HEXANE	317		4.60		C10H5CL7O1	HEPTACHLOR EPOXIDE
3520	CYCLOHEXANE	304		1.20		C10H5F1N2	MALONONITRILE,3-FLUOROBENZAL
3521	CYCLOHEXANE	304		1.22		C10H5F1N2	MALONONITRILE,4-FLUOROBENZAL
3522	CYCLOHEXANE	304		1.55		C10H5F1N2	MALONONITRILE,2-FLUOROBENZAL
3523	OCTANOL	206	27	3.08	3.08 =	C10H5F3N4	QUINOXALINE IMIDAZOLE,2-TRIFLUOROMETHYL
3524	HEXANE	299		0.87		C10H5F3N4O1	CARBONYL CYANIDE,P-TRIFLUOROMETHOXYPHENYLHYDRAZONE
3525	OCTANOL	141		-1.08	-1.08 =	C10H5K1S1O5	1,4-NAPHTHOQUINONE-2-SULFONATE, POTASSIUM SALT
3526	CYCLOHEXANE	304		-0.56		C10H5N1O2	COUMARIN,3-CYANO
3527	CYCLOHEXANE	304		-0.07		C10H5N3O2	MALONONITRILE,3-NITROBENZAL
3528	CYCLOHEXANE	304		-0.02		C10H5N3O2	MALONONITRILE,4-NITROBENZAL
3529	CYCLOHEXANE	304		0.30		C10H5N3O2	MALONONITRILE,2-NITROBENZAL
3530	CYCLOHEXANE	141		0.72		C10H6BR1N1O2	1,4-NAPHTHOQUINONE,2-BROMO,3-AMINO
3531	OCTANOL	141		2.12	2.12 =	C10H6CL1N1O2	1,4-NAPHTHOQUINONE,2-CHLORO-3-AMINO
3532	CYCLOHEXANE	141		0.41		C10H6CL1N1O2	1,4-NAPHTHOQUINONE,2-CHLORO,3-AMINO
3533	OCTANOL	216		2.50	2.50 =	C10H6F3N1	8-TRIFLUOROMETHYLQUINOLINE
3534	OCTANOL	216		2.05	2.05 =	C10H6F3N1O1	4-HYDROXY-7-TRIFLUOROMETHYLQUINOLINE
3535	CYCLOHEXANE	304		1.41		C10H6N2	MALONONITRILE,BENZAL
3536	CYCLOHEXANE	304		-1.62		C10H6N2O1	3-HYDROXYBENZALMALONONITRILE
3537	CYCLOHEXANE	141		-2.15		C10H6N2O1	4-HYDROXYBENZALMALONONITRILE
3538	CYCLOHEXANE	304		-0.06		C10H6O2	1,2-NAPHTHOQUINONE
3539	OCTANOL	238		1.78	1.78 =	C10H6O2	1,4-NAPHTHOQUINONE
3540	OCTANOL	141		1.71	1.71 =	C10H6O2	1,4-NAPHTHOQUINONE
3541	CYCLOHEXANE	141		1.26		C10H6O2	1,4-NAPHTHOQUINONE
3542	OCTANOL	218	26	1.55	1.55 =	C10H6O3	1,4-NAPHTHOQUINONE, 2-HYDROXY
3543	OCTANOL	141		1.38	1.38 =	C10H6O3	1,4-NAPHTHOQUINONE,2-HYDROXY
3544	CYCLOHEXANE	304		-0.56		C10H7CL1N2O1	CYANOACETAMIDE,2-CHLOROBENZAL
3545	CYCLOHEXANE	304		-0.53		C10H7CL1N2O1	CYANOACETAMIDE,4-CHLOROBENZAL
3546	OCTANOL	206		3.19	3.19 =	C10H7CL2F3N2	BENZIMIDAZOLE,2-TRIFLUORMETHYL-4,7-DICL-5,6-DIME
3547	CYCLOHEXANE	304		-1.01		C10H7F1N2O1	CYANOACETAMIDE,2-FLUOROBENZAL
3548	OCTANOL	141		1.88	1.88 =	C10H7N1O2	1,4-NAPHTHOQUINONE, 2-AMINO
3549	CYCLOHEXANE	141		-1.90		C10H7N1O2	1,4-NAPHTHOQUINONE,2-AMINO
3550	CYCLOHEXANE	304		-1.49		C10H7N1O3	COUMARIN,3-CARBAMOYL
3551	OCTANOL	349		3.20	3.20 =	C10H8	AZULENE
3552	OCTANOL	427		3.37	3.37 =	C10H8	NAPHTHALENE
3553	OCTANOL	309		3.01	3.01 =	C10H8	NAPHTHALENE
3554	OCTANOL	428		3.45	3.45 =	C10H8	NAPHTHALENE
3555	CYCLOHEXANE	304		-3.32		C10H8CL2N2O2	MALONAMIDE,2,4-DICHLOROBENZAL
3556	CYCLOHEXANE	304		-1.09		C10H8N2O1	CYANOACETAMIDE,BENZAL
3557	CYCLOHEXANE	141		1.18		C10H8N2O2	STYRENE,3-CYANO,B-NITRO,B-METHYL
3558	CYCLOHEXANE	141		1.18		C10H8N2O2	STYRENE,4-CYANO,B-NITRO,B-METHYL
3559	CHCL3	265		-0.45	0.19 N	C10H8N2O4	A-FURILDIOXIME
3560	OCTANOL	186		2.98	2.98 =	C10H8O1	1-NAPHTHOL
3561	CYCLOHEXANE	325		0.52		C10H8O1	1-NAPHTHOL
3562	OCTANOL	186		2.84	2.84 =	C10H8O1	2-NAPHTHOL
3563	DIETHYL ETHER	359		1.77	1.67 A	C10H8O1	2-NAPHTHOL
3564	CYCLOHEXANE	325		0.29		C10H8O1	2-NAPHTHOL
3565	DIETHYL ETHER	3		-2.00	-1.63 A	C10H8O3S1	NAPHTHALENE SULFONIC ACID
3566	CYCLOHEXANE	304		-3.52		C10H9CL1N2O2	MALONAMIDE,4-CHLOROBENZAL
3567	CYCLOHEXANE	304		-2.69		C10H9CL1N2O2	MALONAMIDE,3-CHLOROBENZAL
3568	CYCLOHEXANE	304		-2.58		C10H9CL1N2O2	MALONAMIDE,2-CHLOROBENZAL
3569	CYCLOHEXANE	141		4.40		C10H9CL2N1O2	STYRENE,2,4-DICHLORO,B-NITRO,B-ETHYL
3570	CYCLOHEXANE	141		4.40		C10H9CL2N1O2	STYRENE,3,4-DICHLORO,B-NITRO,B-ETHYL
3571	CYCLOHEXANE	304		-3.16		C10H9F1N2O2	MALONAMIDE,3-FLUOROBENZAL
3572	CYCLOHEXANE	280		1.64		C10H9N1	2-METHYLQUINOLINE
3573	CYCLOHEXANE	280		1.53		C10H9N1	4-METHYLQUINOLINE
3574	OCTANOL	216		2.57	2.57 =	C10H9N1	6-METHYLQUINOLINE
3575	OCTANOL	216		2.47	2.47 =	C10H9N1	7-METHYLQUINOLINE
3576	OCTANOL	216		2.60	2.60 =	C10H9N1	8-METHYLQUINOLINE
3577	CYCLOHEXANE	280		2.22		C10H9N1	8-METHYLQUINOLINE
3578	BENZENE	72		2.40	2.22 B	C10H9N1	A-NAPHTHYLAMINE
3579	PARAFFINS	316		0.99		C10H9N1	A-NAPHTHYLAMINE
3580	BENZENE	72		2.45	2.25 B	C10H9N1	B-NAPHTHYLAMINE
3581	PARAFFINS	316		0.98		C10H9N1	B-NAPHTHYLAMINE
3582	OCTANOL	216		2.20	2.20 =	C10H9N1O1	6-METHOXYQUINOLINE
3583	OCTANOL	216		1.84	1.84 =	C10H9N1O1	8-METHOXYQUINOLINE
3584	OCTANOL	410		2.33	2.33 =	C10H9N1O1	8-QUINOLINOL,2-METHYL
3585	OCTANOL	410		2.41	2.41 =	C10H9N1O1	8-QUINOLINOL,4-METHYL
3586	CHCL3	412		3.22	2.56 B	C10H9N1O1	8-QUINOLINOL,2-METHYL
3587	CHCL3	412		3.27	2.57 B	C10H9N1O1	8-QUINOLINOL,4-METHYL
3588	N-BUTANOL	410		1.92	2.15	C10H9N1O1	8-QUINOLINOL,2-METHYL
3589	N-BUTANOL	410		1.96	2.21	C10H9N1O1	8-QUINOLINOL,4-METHYL
3590	TOLUENE	410		2.75	2.67 B	C10H9N1O1	8-QUINOLINOL,2-METHYL
3591	TOLUENE	410		2.77	2.69 B	C10H9N1O1	8-QUINOLINOL,4-METHYL
3592	PRIM. PENTANOLS	410		2.13	2.40	C10H9N1O1	8-QUINOLINOL,2-METHYL
3593	PRIM. PENTANOLS	410		2.19	2.47	C10H9N1O1	8-QUINOLINOL,4-METHYL
3594	1-PENT. ACETATE	410		2.61	2.53	C10H9N1O1	8-QUINOLINOL,2-METHYL
3595	I-PENT. ACETATE	410		2.69	2.61	C10H9N1O1	8-QUINOLINOL,4-METHYL
3596	CCL4	412		2.64	2.34 B	C10H9N1O1	8-QUINOLINOL,2-METHYL
3597	CCL4	412		2.73	2.41 B	C10H9N1O1	8-QUINOLINOL,4-METHYL
3598	ME-I-BUT.KETONE	410		2.50	2.27	C10H9N1O1	8-QUINOLINOL,2-METHYL
3599	ME-I-BUT.KETONE	410		2.63	2.45	C10H9N1O1	8-QUINOLINOL,4-METHYL
3600	O-DICL. BENZENE	410		3.00		C10H9N1O1	8-QUINOLINOL,2-METHYL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3601	O-DICL. BENZENE	410		3.01		C10H9N1O1	8-QUINOLINOL,4-METHYL
3602	OCTANOL	218		1.41	1.41 =	C10H9N1O2	INDOLE-3-ACETIC ACID
3603	DIETHYL ETHER	3		1.30	1.26 A	C10H9N1O2	INDOLE-3-ACETIC ACID
3604	HEXANE	376		0.21		C10H9N1O2S1	N-METHYLCARBAMIC ACID,4-BENZOTHIENYL ESTER
3605	CYCLOHEXANE	141		2.06		C10H9N1O4	STYRENE,3,4-DIOXYMETHYLENE,B-NITRO,B-METHYL
3606	OCTANOL	65	46	-2.64	-2.64 =	C10H10BR1N1	N-METHYLQUINOLINIUM BROMIDE
3607	CYCLOHEXANE	141		2.92		C10H10BR1N1O3	STYRENE,5-BROMO,2-METHOXY,B-NITRO,B-METHYL
3608	CYCLOHEXANE	141		3.19		C10H10CL1N1O2	STYRENE,4-CHLORO,B-NITRO,B-ETHYL
3609	CYCLOHEXANE	141		3.23		C10H10CL1N1O2	STYRENE,2-CHLORO,B-NITRO,B-ETHYL
3610	CYCLOHEXANE	141		4.40		C10H10CL1N1O2	STYRENE,3-CHLORO,B-NITRO,B-ETHYL
3611	OILS	383		-0.60	0.67 A	C10H10CL1N1O3	P-AMINOPHENYLACETIC ACID,N-CHLOROACETYL
3612	CYCLOHEXANE	141		3.02		C10H10CL1N1O3	STYRENE,5-CHLORO,2-METHOXY,B-NITRO,B-METHYL
3613	OCTANOL	346		0.67	0.67 =	C10H10CL1N1O4	PHENOXYACETIC ACID,3-ACETAMIDO-4-CHLORO
3614	OCTANOL	302		0.75	0.75 =	C10H10CL1N1O4	PHENOXYACETIC ACID,3-ACETAMIDO-4-CHLORO
3615	HEXANE	391		2.07		C10H10CL3O4P1	2-CL-1-(2,5-DICLPHENYL)-VINYLPHOSPHATE,O,O-DIME
3616	HEXANE	391		2.43		C10H10CL3O4P1	2-CL-1-(2,4-DICLPHENYL)-VINYLPHOSPHATE,O,O-DIME
3617	OCTANOL	227		-0.48	-0.48 =	C10H10F3N2O5	2'-DEOXY-5-TRIFLUOROMETHYLURIDINE(75520)(PKA=7.95)
3618	DIETHYL ETHER	306		1.18	1.20 A	C10H10I1N1O6S1	N-(P-IODOBENZENESULFONYL)ASPARTIC ACID
3619	CHCL3	306	12	-2.00	-0.58 A	C10H10I1N1O6S1	N-(P-IODOBENZENESULFONYL)ASPARTIC ACID
3620	ETHYL ACETATE	306	12	1.95	2.04 A	C10H10I1N1O6S1	N-(P-IODOBENZENESULFONYL)ASPARTIC ACID
3621	CLCH2CH2CL	306		-1.30		C10H10I1N1O6S1	N-(P-IODOBENZENESULFONYL)ASPARTIC ACID
3622	OILS	382	24	4.50	5.28 A	C10H10I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,PROPYL ESTER
3623	OILS	382	24	2.10	3.10 A	C10H10I2O4	BENZOIC ACID,3,5-DI-IODO-4-OH,B-OH-PROPYL ESTER
3624	OILS	382	24	2.18	3.17 A	C10H10I2O4	BENZOIC ACID,4-OH,3,5-DI-IODO,G-OH-PROPYL ESTER
3625	CYCLOHEXANE	304		-3.46		C10H10N2O2	MALONAMIDE,BENZAL
3626	CYCLOHEXANE	141		2.39		C10H10N2O4	STYRENE,4-NITRO,B-NITRO,B-ETHYL
3627	OCTANOL	134		1.66	1.66 =	C10H10N4O1S1	3-METHIO-4-AMINO-6-PHENYL-1,2,4-TRIAZINE-5-ONE
3628	OCTANOL	393	63	-0.13	-0.13 =	C10H10N4O2S1	SULFADIAZINE
3629	OCTANOL	56		-0.08	-0.08 =	C10H10N4O2S1	SULFADIAZINE
3630	DIETHYL ETHER	342		-0.48	-0.32 A	C10H10N4O2S1	SULFADIAZINE
3631	CHCL3	343	2	0.06	-0.18 B	C10H10N4O2S1	SULFADIAZINE
3632	CHCL3	326		-0.03	-0.26 B	C10H10N4O2S1	SULFADIAZINE
3633	CHCL3	344	44	-0.40	-0.45 B	C10H10N4O2S1	SULFADIAZINE
3634	CHCL3	393	63	0.22	0.20 N	C10H10N4O2S1	SULFADIAZINE
3635	BENZENE	343	2	-0.89	-0.07 B	C10H10N4O2S1	SULFADIAZINE
3636	1-BUTANOL	130	13	0.12	-0.34	C10H10N4O2S1	SULFADIAZINE
3637	1-PENT. ACETATE	343	2	0.19	0.02	C10H10N4O2S1	SULFADIAZINE
3638	CCL4	343	2	-2.22	-0.00 A	C10H10N4O2S1	SULFADIAZINE
3639	N-BUTANOL	253	36	0.79	0.61	C10H10N6	4,6-DIAMINO-5-PHENYLAZOPYRIMIDINE
3640	CYCLOHEXANE	304		1.50		C10H10O1	METHYL STYRYL KETONE
3641	CHCL3	429		3.60	4.50 A	C10H10O2	BENZOYLACETONE
3642	CHCL3	387		3.44	4.32 A	C10H10O2	BENZOYLACETONE
3643	BENZENE	429	5	3.15	4.50 A	C10H10O2	BENZOYLACETONE
3644	BENZENE	387		3.14	4.41 A	C10H10O2	BENZOYLACETONE
3645	CCL4	429		2.82	4.27 A	C10H10O2	BENZOYLACETONE
3646	DIETHYL ETHER	3		1.18	1.15 A	C10H10O4	BENZYLMALONIC ACID
3647	1-BUTANOL	4		1.48	1.57	C10H10O4	BENZYLMALONIC ACID
3648	OCTANOL	10		0.87	0.87 =	C10H10O4	PHENOXYACETIC ACID,4-ACETYL
3649	OCTANOL	10		0.98	0.98 =	C10H10O4	PHENOXYACETIC ACID,3-ACETYL
3650	OCTANOL	10		1.25	1.25 =	C10H10O4	PHENOXYACETIC ACID,2-ACETYL
3651	50%ETHER+50%DMF	125		0.16	1.20	C10H11BR1N2O3	BARBITURIC ACID, 5-ALLYL-5-(2-BROMALLYL)
3652	OCTANOL	430	46	-0.05	-0.05 =	C10H11CL1N2.H3PO7	5-CHLOROTRYPTAMINE PHOSPHATE
3653	OCTANOL	255		2.21	2.21 =	C10H11N1	BENZENE,3-CYANO-1-PROPYL
3654	OCTANOL	309		2.82	2.82 =	C10H11N1	INDOLE, 1,2-DIMETHYL
3655	I-PENT. ACETATE	418	3	2.70	2.62	C10H11N1O2	P-AMINOBENZOIC ACID,ALLYL ESTER
3656	OCTANOL	141		2.86	2.86 =	C10H11N1O2	BENZENE, 2-NITRO-1-BUTENYL
3657	CYCLOHEXANE	141		3.45		C10H11N1O2	STYRENE,B-ETHYL,B-NITRO
3658	CYCLOHEXANE	141		2.98		C10H11N1O2	STYRENE,2-METHYL,B-NITRO,B-METHYL
3659	CYCLOHEXANE	141		3.00		C10H11N1O2	STYRENE,4-METHYL,B-NITRO,B-METHYL
3660	CHCL3	394		2.00	1.48 B	C10H11N1O3	P-ACETOXYACETANILIDE
3661	OILS	383		-0.55	0.71 A	C10H11N1O3	P-AMINOPHENYLACETIC ACID,N-ACETYL
3662	HEXANE	376		1.20		C10H11N1O3	N-METHYL-N-ACETYLCARBAMIC ACID,PHENYL ESTER
3663	OCTANOL	384		0.90	0.90 =	C10H11N1O3	N-METHYL-3-ACETYLPHENYLCARBAMATE
3664	CYCLOHEXANE	141		2.33		C10H11N1O3	STYRENE,4-METHOXY,B-NITRO,B-METHYL
3665	CYCLOHEXANE	141		2.61		C10H11N1O3	STYRENE,2-METHOXY,B-NITRO,B-METHYL
3666	CYCLOHEXANE	141		2.63		C10H11N1O3	STYRENE,3-METHOXY,B-NITRO,B-METHYL
3667	DIETHYL ETHER	431		-1.00	-0.75 A	C10H11N1O4	BENZOYLSERINE
3668	OCTANOL	384		1.42	1.42 =	C10H11N1O4	N-METHYL-3-CARBOMETHOXYPHENYLCARBAMATE
3669	OCTANOL	384		1.50	1.50 =	C10H11N1O4	N-METHYL-4-CARBOMETHOXYPHENYLCARBAMATE
3670	OCTANOL	10		0.48	0.48 =	C10H11N1O4	PHENOXYACETIC ACID,M-ACETAMIDO
3671	CYCLOHEXANOL	302		1.27		C10H11N1O4	PHENOXYACETIC ACID,M-ACETAMIDO
3672	CYCLOHEXANE	141		0.88		C10H11N1O4	STYRENE,3,4-DIMETHOXY,B-NITRO
3673	CYCLOHEXANE	141		1.79		C10H11N1O4	STYRENE,2,5-DIMETHOXY,B-NITRO
3674	CYCLOHEXANE	141		1.93		C10H11N1O4	STYRENE,2,3-DIMETHOXY,B-NITRO
3675	CYCLOHEXANE	141		2.04		C10H11N1O4	STYRENE,2,4-DIMETHOXY,B-NITRO
3676	CYCLOHEXANE	141		0.77		C10H11N1O4	STYRENE,4-HYDROXY,3-METHOXY,B-NITRO,B-METHYL
3677	OCTANOL	393	63	0.88	0.88 =	C10H11N3O3S1	SULFAMETHOXAZOLE
3678	CHCL3	343	2	0.55	1.10 N	C10H11N3O3S1	SULFAMETHOXAZOLE
3679	CHCL3	393	63	0.52	1.08 N	C10H11N3O3S1	SULFAMETHOXAZOLE
3680	BENZENE	343	2	-0.19	1.22 A	C10H11N3O3S1	SULFAMETHOXAZOLE
3681	1-PENT. ACETATE	343	2	1.34	1.21	C10H11N3O3S1	SULFAMETHOXAZOLE
3682	CCL4	343	2	-1.49	0.60 A	C10H11N3O3S1	SULFAMETHOXAZOLE
3683	HEXANE	391		0.99		C10H12CL1N1O2	N-METHYL CARBAMATE,3,4-DIMETHYL,6-CHLOROPHENYL
3684	HEXANE	391		1.46		C10H12CL1N1O2	N-METHYL CARBAMATE,3,5-DIMETHYL,4-CHLOROPHENYL
3685	N-HEPTANE	416	14	0.84		C10H12CL1N1O3	P-AMINOSALICYLIC ACID, 3-CHLOROPROPYL ESTER
3686	N-HEPTANE	138		1.23		C10H12F3N1	NORFENFLURAMINE
3687	DIETHYL ETHER	306		0.90	0.95 A	C10H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)THREONINE
3688	CHCL3	306		-0.80	0.48 A	C10H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)THREONINE
3689	ETHYL ACETATE	306		1.65	1.70 A	C10H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)THREONINE
3690	CLCH2CH2CL	306		-0.39		C10H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)THREONINE
3691	OLEYL ALCOHOL	406		2.85	3.42	C10H12N1O2S1	N-TRICLMETHIO-4-METHYLHEXAHYDROPHTHALIMIDE
3692	ETHYL ACETATE	432		1.41	1.46	C10H12N2	3-(2-AMINOETHYL)INDOLE/TRYPTAMINE/
3693	OCTANOL	341	60	1.13	1.13 =	C10H12N2	DIHYDRONICOTYRINE
3694	OCTANOL	430	46	-1.02	-1.02 =	C10H12N2.H3PO4	TRYPTAMINE PHOSPHATE
3695	OCTANOL	218		0.21	0.21 =	C10H12N2O1	5-HYDROXY-3-(2-AMINOETHYL)INDOLE
3696	ETHYL ACETATE	432		0.61	0.60	C10H12N2O1	5-HYDROXY-3-(2-AMINOETHYL)INDOLE
3697	OCTANOL	276		1.25	1.25 =	C10H12N2O1	2-(G-HYDROXYPROPYL)-BENZIMIDAZOLE
3698	OCTANOL	430	46	-1.77	-1.77 =	C10H12N2O1.H3PO4	5-HYDROXYTRYPTAMINE PHOSPHATE
3699	OCTANOL	141		2.67	2.67 =	C10H12N2O2	STYRENE, 4-DIMETHYLAMINO-B-NITRO
3700	CYCLOHEXANE	141		1.94		C10H12N2O2	STYRENE,4-DIMETHYLAMINO,B-NITRO

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3701	OCTANOL	399		1.19	1.19 =	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3702	CHCL3	399	1	0.33	0.89 N	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3703	OILS	345		-0.07	1.13 A	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3704	OILS	296		-0.12	1.08 A	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3705	OILS	168		-0.07	1.13 A	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3706	BENZENE	399	1	-0.35	1.07 A	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3707	1-PENT. ACETATE	399	1	1.23	1.10	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3708	CCL4	399	1	-0.96	1.05 A	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3709	OLEYL ALCOHOL	82		0.38	0.94	C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3710	MIXED SOLV#1	433		0.38		C10H12N2O3	BARBITURIC ACID,DIALLYL/DIAL/
3711	50%ETHER+50%DMF	125		0.23	1.35	C10H12N2O3	BARBITURIC ACID, DIALLYL/DIAL/
3712	HEXANE	391		1.87		C10H12N3O3P1S2	METHYLAZINPHOS/GUTHION/
3713	CHCL3	343	2	0.49	1.10 N	C10H12N4O2S2	SULFAETHIDOLE
3714	CHCL3	415	44	0.09	0.69 N	C10H12N4O2S2	SULFAETHIDOLE
3715	BENZENE	343	2	-0.66	0.77 A	C10H12N4O2S2	SULFAETHIDOLE
3716	1-PENT. ACETATE	343	2	0.90	0.76	C10H12N4O2S2	SULFAETHIDOLE
3717	CCL4	343	2	-1.27	0.78 A	C10H12N4O2S2	SULFAETHIDOLE
3718	N-HEPTANE	415	44	-2.54		C10H12N4O2S2	SULFAETHIDOLE
3719	OCTANOL	227		-0.60	-0.60 =	C10H12N4O4S1	6-MERCAPTOPURINE RIBOSIDE (4911)
3720	OCTANOL	227		-0.57	-0.57 =	C10H12N4O4S1	9H-PURINE-6-THIOL,9-B-D-ARABINOFURANOSYL (PKA= 787)
3721	OCTANOL	277	14	-2.08	-2.08 =	C10H12N4O5	INOSINE
3722	N-BUTANOL	253	36	-0.92	-1.79	C10H12N4O5	INOSINE
3723	N-BUTANOL	253	36	-1.30	-2.32	C10H12N4O6	XANTHOSINE
3724	CYCLOHEXANE	325		0.97		C10H12O1	4-INDANOL,1-METHYL
3725	CYCLOHEXANE	325		1.00		C10H12O1	4-INDANOL,6-METHYL
3726	CYCLOHEXANE	325		1.06		C10H12O1	4-INDANOL,7-METHYL
3727	CYCLOHEXANE	325		1.21		C10H12O1	4-INDANOL,5-METHYL
3728	CYCLOHEXANE	325		0.87		C10H12O1	5-INDANOL,7-METHYL
3729	OCTANOL	56		1.95	1.95 =	C10H12O1	TR-2-PHENYLCYCLOPROPYLCARBINOL
3730	OCTANOL	255		2.30	2.30 =	C10H12O2	ACETIC ACID,B-PHENYLETHYL ESTER
3731	OILS	383		1.56	2.65 A	C10H12O2	P-ETHYLPHENYLACETIC ACID
3732	OILS	327		1.99	2.99 A	C10H12O2	PHENOL,2-METHOXY-4-ALLYL/EUGENOL/
3733	PARAFFINS	327		1.34		C10H12O2	PHENOL,2-METHOXY-4-ALLYL/EUGENOL/
3734	OILS	362		0.74	1.89 A	C10H12O2	A-PHENYLBUTYRIC ACID
3735	OILS	385		1.16	2.25 A	C10H12O2	A-PHENYLBUTYRIC ACID
3736	OILS	417		1.06	2.15 A	C10H12O2	B-PHENYLBUTYRIC ACID
3737	OCTANOL	255		2.42	2.42 =	C10H12O2	4-PHENYLBUTYRIC ACID
3738	OILS	361		0.92	2.08 A	C10H12O2	4-PHENYLBUTYRIC ACID
3739	OILS	417		1.17	2.35 A	C10H12O2	4-PHENYLBUTYRIC ACID
3740	OCTANOL	255		2.32	2.32 =	C10H12O2	B-PHENYLPROPIONIC ACID,METHYL ESTER
3741	OILS	383		0.92	2.06 A	C10H12O3	P-ETHOXYPHENYLACETIC ACID
3742	OCTANOL	56		3.04	3.04 =	C10H12O3	P-HYDROXYBENZOIC ACID,PROPYL ESTER
3743	OCTANOL	10		2.25	2.25 =	C10H12O3	PHENOXYACETIC ACID,3-ETHYL
3744	OCTANOL	10		2.65	2.65 =	C10H12O3	PHENOXYACETIC ACID,2-ETHYL
3745	CYCLOHEXANOL	302		2.55		C10H12O3	PHENOXYACETIC ACID,3-ETHYL
3746	50%ETHER+50%DMF	125		0.32	1.60	C10H13BR1N2O3	BARBITURIC ACID,5-(2-BROMALLYL)-5-I-PROPYL
3747	OCTANOL	227		2.90	2.90 =	C10H13CL2N1	N,N-DI-B-CHLOROETHYLANILINE
3748	DIETHYL ETHER	374		1.46	2.16 B	C10H13N1	N-METHYL-1-PHENYLPROPYLAMINE-2
3749	OCTANOL	255		1.41	1.41 =	C10H13N1O1	BUTYRAMIDE,4-PHENYL
3750	OCTANOL	186		1.58	1.58 =	C10H13N1O2	ACETANILIDE,4-ETHOXY/PHENACETIN/
3751	OILS	173		0.43	1.58 A	C10H13N1O2	ACETANILIDE,4-ETHOXY/PHENACETIN/
3752	OILS	224		0.60	1.77 A	C10H13N1O2	ACETANILIDE,4-ETHOXY/PHENACETIN/
3753	1-PENT. ACETATE	418	3	2.81	2.73	C10H13N1O2	P-AMINOBENZOIC ACID,1-PROPYL ESTER
3754	1-PENT. ACETATE	418	3	3.17	3.10	C10H13N1O2	P-AMINOBENZOIC ACID,N-PROPYL ESTER
3755	OLEYL ALCOHOL	390	44	2.28	2.82	C10H13N1O2	P-AMINOBENZOIC ACID,PROPYL ESTER
3756	OCTANOL	276		1.00	1.00 =	C10H13N1O2	M-METHOXY-N,N-DIMETHYLBENZAMIDE
3757	OCTANOL	276		0.71	0.71 =	C10H13N1O2	O-METHOXY-N,N-DIMETHYLBENZAMIDE
3758	OCTANOL	276		0.96	0.96 =	C10H13N1O2	P-METHOXY-N,N-DIMETHYLBENZAMIDE
3759	HEXANE	391		0.56		C10H13N1O2	N-METHYL CARBAMATE,3,5-DIMETHYLPHENYL
3760	HEXANE	391		0.60		C10H13N1O2	N-METHYL CARBAMATE,3,4-DIMETHYLPHENYL
3761	HEXANE	391		0.61		C10H13N1O2	N-METHYL CARBAMATE,3-ETHYLPHENYL
3762	OCTANOL	384		1.93	1.93 =	C10H13N1O2	N-METHYL-2-ETHYLPHENYLCARBAMATE
3763	OCTANOL	384		1.95	1.95 =	C10H13N1O2	N-METHYL-2,3-DIMETHYLPHENYLCARBAMATE
3764	OCTANOL	384		2.03	2.03 =	C10H13N1O2	N-METHYL-2,5-DIMETHYLPHENYLCARBAMATE
3765	OCTANOL	384		2.20	2.20 =	C10H13N1O2	N-METHYL-3-ETHYLPHENYLCARBAMATE
3766	OCTANOL	384		2.09	2.09 =	C10H13N1O2	N-METHYL-3,4-DIMETHYLPHENYLCARBAMATE
3767	OCTANOL	384		2.23	2.23 =	C10H13N1O2	N-METHYL-3,5-DIMETHYLPHENYLCARBAMATE
3768	OCTANOL	384		2.23	2.23 =	C10H13N1O2	N-METHYL-4-ETHYLPHENYLCARBAMATE
3769	HEXANE	391		0.62		C10H13N1O2S1	N-METHYL CARBAMATE,3-METHYL,4-METHYLTHIOPHENYL
3770	OCTANOL	384		2.47	2.47 =	C10H13N1O2S1	N-METHYL-3-METHYL-4-METHYLTHIOPHENYLCARBAMATE
3771	N-HEPTANE	370	14	1.02		C10H13N1O3	P-AMINOSALICYLIC ACID,N-PROPYL ESTER
3772	OCTANOL	384		1.24	1.24 =	C10H13N1O3	N-METHYL-2-ETHOXYPHENYLCARBAMATE
3773	OCTANOL	384		1.75	1.75 =	C10H13N1O3	N-METHYL-3-ETHOXYPHENYLCARBAMATE
3774	OCTANOL	384		1.63	1.63 =	C10H13N1O3	N-METHYL-4-ETHOXYPHENYLCARBAMATE
3775	N-HEPTANE	370	14	-0.68		C10H13N1O4	P-AMINOSALICYLIC ACID,3-HYDROXYPROPYL ESTER
3776	OCTANOL	227		-0.56	-0.56 =	C10H13N5O3S1	B-2'-DEOXYTHIOGUANOSINE (71261)
3777	OCTANOL	227		-0.79	-0.79 =	C10H13N5O3S1	A-2'-DEOXYTHIOGUANOSINE (71851)
3778	OCTANOL	277	14	-1.10	-1.10 =	C10H13N5O4	ADENOSINE
3779	OCTANOL	218		-1.23	-1.23 =	C10H13N5O4	ADENOSINE
3780	N-BUTANOL	253	36	-0.18	-0.76	C10H13N5O4	ADENOSINE
3781	N-BUTANOL	253	36	-0.92	-1.79	C10H13N5O5	GUANOSINE
3782	OCTANOL	56		4.11	4.11 =	C10H14	BENZENE, T-BUTYL
3783	OCTANOL	298		4.11	4.11 =	C10H14	BENZENE, T-BUTYL
3784	CHCL3	396	31	2.90	2.26 B	C10H14CL1N1	CHLORPHENTERMINE
3785	N-HEPTANE	396	31	1.24		C10H14CL1N1	CHLORPHENTERMINE
3786	OCTANOL	392		2.15	2.15 =	C10H14N1O5P1S1	PARATHION
3787	OCTANOL	392		1.69	1.69 =	C10H14N1O6P1	PARA-OXON
3788	OCTANOL	341	60	0.97	0.97 =	C10H14N2	ANABASINE
3789	DIETHYL ETHER	434		-0.23	0.66 B	C10H14N2	ANABASINE
3790	CYCLOHEXANE	434		-0.58		C10H14N2	ANABASINE
3791	CHCL3	434		0.82	0.54 B	C10H14N2	ANABASINE
3792	BENZENE	434		0.30	0.76 B	C10H14N2	ANABASINE
3793	TOLUENE	434		0.20	0.81 B	C10H14N2	ANABASINE
3794	CCL4	434		-0.01		C10H14N2	ANABASINE
3795	CLCH2CH2CL	434		0.52		C10H14N2	ANABASINE
3796	PARAFFINS	434		-0.60		C10H14N2	ANABASINE
3797	OCTANOL	341	60	1.13	1.13 =	C10H14N2	4-(N-METHYL)-3-PRYIDYLBUTENE-1-YLAMINE
3798	OCTANOL	341	60	1.17	1.17 =	C10H14N2	NICOTINE
3799	CYCLOHEXANE	435		0.25		C10H14N2	NICOTINE
3800	CHCL3	435		1.89	1.38 B	C10H14N2	NICOTINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3801	BENZENE	435		0.98	1.23 B	C10H14N2	NICOTINE
3802	XYLENE	435		0.75	1.41 B	C10H14N2	NICOTINE
3803	TOLUENE	435		0.86	1.25 B	C10H14N2	NICOTINE
3804	NITROBENZENE	435		0.91	1.62	C10H14N2	NICOTINE
3805	N-BUTYL ACETATE	435		0.78	1.06	C10H14N2	NICOTINE
3806	CCL4	435		0.94	0.80 B	C10H14N2	NICOTINE
3807	CLCH2CH2CL	435		1.17		C10H14N2	NICOTINE
3808	N-HEPTANE	435		0.03		C10H14N2	NICOTINE
3809	N-HEPTANE	400	14	-0.80		C10H14N2	NICOTINE
3810	O-DICL. BENZENE	435		1.03		C10H14N2	NICOTINE
3811	PARAFFINS	435		0.05		C10H14N2	NICOTINE
3812	OCTANOL	341	60	1.10	1.10 =	C10H14N2	3-PYRIDYLMETHYL-N-PYRROLIDINE
3813	OCTANOL	218		0.33	0.33 =	C10H14N2O1	NIKETHAMIDE
3814	OCTANOL	341	60	0.04	0.04 =	C10H14N2O1	3-PYRIDYLMETHYL-N-MORPHOLINE
3815	N-HEPTANE	419		-0.85		C10H14N2O1	UREA,ETHYL,M-TOLYL-
3816	N-HEPTANE	419		-1.18		C10H14N2O1	UREA,ETHYL,O-TOLYL-
3817	N-HEPTANE	419		-0.89		C10H14N2O1	UREA,ETHYL,P-TOLYL-
3818	N-HEPTANE	419		-1.80		C10H14N2O1	UREA,METHYL,O-PHENETYL-
3819	N-HEPTANE	419		-0.96		C10H14N2O1	UREA,N-PROPYLPHENYL-
3820	OCTANOL	384		1.43	1.43 =	C10H14N2O2	N-METHYL-3-DIMETHYLAMINOPHENYLCARBAMATE
3821	N-HEPTANE	419		-1.66		C10H14N2O2	UREA,ETHYL,O-ANISYL-
3822	N-HEPTANE	419		-1.55		C10H14N2O2	UREA,ETHYL,P-ANISYL-
3823	OCTANOL	218		2.19	2.19 =	C10H14N2O2S1	BARBITURIC ACID,5-ETHYL-5-METHYLALLYL-2-THIO
3824	OILS	345		0.05	1.24 A	C10H14N2O3	BARBITURIC ACID, 5-ALLYL-5-I-PROPYL
3825	OILS	371		0.24	0.64 B	C10H14N4O3	CAFFEINE,ETHOXY
3826	OCTANOL	181	10	-0.22	-0.22 =	C10H14N5O7P1	3-ADENYLIC ACID
3827	N-BUTANOL	181	10	-0.52		C10H14N5O7P1	3-ADENYLIC ACID
3828	PRIM. PENTANOLS	181	10	-0.10		C10H14N5O7P1	3-ADENYLIC ACID
3829	HEXANOL	181	18	-0.22		C10H14N5O7P1	3-ADENYLIC ACID
3830	OCTANOL	181	10	0.28	0.28 =	C10H14N5O7P1	5-ADENYLIC ACID
3831	N-BUTANOL	181	10	-0.70		C10H14N5O7P1	5-ADENYLIC ACID
3832	PRIM. PENTANOLS	181	10	-0.40		C10H14N5O7P1	5-ADENYLIC ACID
3833	HEXANOL	181	18	-0.30		C10H14N5O7P1	5-ADENYLIC ACID
3834	OCTANOL	181	10	0.68	0.68 =	C10H14N5O8P1	GUANYLIC ACID
3835	N-BUTANOL	181	10	-0.70		C10H14N5O8P1	GUANYLIC ACID
3836	PRIM. PENTANOLS	181	10	-0.40		C10H14N5O8P1	GUANYLIC ACID
3837	HEXANOL	181	18	-0.40		C10H14N5O8P1	GUANYLIC ACID
3838	HEXANE	372		0.51		C10H14O1	BUTANOL,4-PHENYL
3839	OCTANOL	56		3.31	3.31 =	C10H14O1	P-T-BUTYLPHENOL
3840	CYCLOHEXANE	325		1.12		C10H14O1	P-T-BUTYLPHENOL
3841	CYCLOHEXANE	325		1.29		C10H14O1	P-T-BUTYLPHENOL
3842	OCTANOL	65		1.97	1.97 =	C10H14O1	2-DECALONE
3843	CYCLOHEXANE	325		1.30		C10H14O1	PHENOL,2-METHYL,5-I-PROPYL
3844	OCTANOL	255		2.70	2.70 =	C10H14O1	PROPANE, 1-METHOXY-3-PHENYL
3845	OCTANOL	186		3.30	3.30 =	C10H14O1	THYMOL
3846	OILS	173		2.79	3.73 A	C10H14O1	THYMOL
3847	OILS	82		2.78	3.72 A	C10H14O1	THYMOL
3848	OILS	436		2.65	3.68 A	C10H14O1	THYMOL
3849	OLEYL ALCOHOL	82		2.98	3.52	C10H14O1	THYMOL
3850	OCTANOL	186		1.52	1.52 =	C10H14O2	CAMPHORQUINONE
3851	OILS	327		2.16	3.15 A	C10H14O2	PHENOL,2-METHOXY-4-PROPYL/P-PROPYLGUAIACOL/
3852	PARAFFINS	327		1.78		C10H14O2	PHENOL,2-METHOXY-4-PROPYL/P-PROPYLGUAIACOL
3853	OCTANOL	218		1.41	1.41 =	C10H14O3	1,2-PROPANEDIOL, 3-(2-TOLYLOXY)
3854	OCTANOL	373		-1.39	-1.39 =	C10H15CL1N2O1	N1-BUTYLNICOTINAMIDE CHLORIDE
3855	DIETHYL ETHER	374		1.49	2.17 B	C10H15N1	BENZYLPROPYLAMINE
3856	XYLENE	422		1.32	1.96 B	C10H15N1	1-BENZYLPROPYLAMINE
3857	OCTANOL	312	12	3.58	3.58 =	C10H15N1	N-BUTYLANILINE
3858	CHCL3	396	31	2.75	2.12 B	C10H15N1	METHAMPHETAMINE/DESOXYEPHEDRINE/
3859	XYLENE	422		1.58	2.23 B	C10H15N1	METHAMPHETAMINE/DESOXYEPHEDRINE/
3860	N-HEPTANE	138		1.24		C10H15N1	METHAMPHETAMINE/DESOXYEPHEDRINE/
3861	N-HEPTANE	396	31	0.71		C10H15N1	METHAMPHETAMINE/DESOXYEPHEDRINE/
3862	DIETHYL ETHER	374		1.46	2.14 B	C10H15N1	N-METHYL-G-PHENYLPROPYLAMINE
3863	N-HEPTANE	421	44	1.63		C10H15N1	PHENETHYLDIMETHYLAMINE
3864	CHCL3	396	31	2.71	2.10 B	C10H15N1	PHENTERMINE
3865	N-HEPTANE	396	31	1.80		C10H15N1	PHENTERMINE
3866	OCTANOL	218		0.93	0.93 =	C10H15N1O1	EPHEDRINE
3867	DIETHYL ETHER	3		0.30	1.12 B	C10H15N1O1	EPHEDRINE
3868	CYCLOHEXANE	357		-0.39		C10H15N1O1	EPHEDRINE
3869	CHCL3	405	31	1.05	0.75 B	C10H15N1O1	EPHEDRINE
3870	CHCL3	396	31	0.38	0.10 B	C10H15N1O1	EPHEDRINE
3871	1-BUTANOL	4		1.18	1.15	C10H15N1O1	EPHEDRINE
3872	N-HEPTANE	396	31	-3.00		C10H15N1O1	EPHEDRINE
3873	CHCL3	396	31	1.30	0.89 B	C10H15N1O1	PSEUDOEPHEDRINE
3874	N-HEPTANE	396	31	-1.54		C10H15N1O1	PSEUDOEPHEDRINE
3875	DIETHYL ETHER	113		2.22	2.05 A	C10H15N1O2S1	N,N-DIETHYLBENZENESULFONAMIDE
3876	CHCL3	113		3.65	4.08 N	C10H15N1O2S1	N,N-DIETHYLBENZENESULFONAMIDE
3877	OCTANOL	397		1.79	1.79 =	C10H15N5	ADENINE,9-PENTYL
3878	OCTANOL	397		0.66	0.66 =	C10H15N5O1	ADENINE,9-(1-HYDROXYMETHYL-BUTYL)
3879	OCTANOL	181	10	0.89	0.89 =	C10H15N5O10P2	ADP
3880	N-BUTANOL	181	10	-0.52		C10H15N5O10P2	ADP
3881	PRIM. PENTANOLS	181	10	0.85		C10H15N5O10P2	ADP
3882	HEXANOL	181	18	0.71		C10H15N5O10P2	ADP
3883	OCTANOL	437		3.46	3.46 =	C10H15O3P1S1	O,O-DIETHYL-O-PHENYLPHOSPHOROTHIOATE
3884	OCTANOL	437		1.64	1.64 =	C10H15O4P1	O,O-DIETHYL-O-PHENYLPHOSPHATE
3885	OCTANOL	341	60	1.34	1.34 =	C10H16N2	N-BUTYL-3-PYRIDYLMETHYLAMINE
3886	OCTANOL	341	60	1.01	1.01 =	C10H16N2	N,N-DIETHYL-3-PYRIDYLMETHYLAMINE
3887	OCTANOL	341	60	0.91	0.91 =	C10H16N2	4-(N-METHYL)-3-PYRIDYLBUTYLAMINE
3888	50%ETHER+50%DMF	125		0.71	2.57	C10H16N2O2S1	5-S-BUTYL-5-ET-2-THIOBARBITURIC ACID/INACTIN/
3889	OCTANOL	218		1.89	1.89 =	C10H16N2O3	BARBITURIC ACID,5-BUTYL-5-ETHYL
3890	OILS	345		0.41	1.56 A	C10H16N2O3	BARBITURIC ACID,5-BUTYL-5-ETHYL
3891	OILS	345		0.13	1.31 A	C10H16N2O3	BARBITURIC ACID,5-ETHYL-5-S-BUTYL
3892	50%ETHER+50%DMF	125		0.29	1.52	C10H16N2O3	BARBITURIC ACID, 5-S-BUTYL-5-ETHYL
3893	OCTANOL	134		2.14	2.14 =	C10H16N4O1S1	3-METHIO-4-AMINO-6-CYCLOHEXYL-1,2,4-TRIAZINE-5-ONE
3894	OCTANOL	181	10	1.64	1.64 =	C10H16N5O13P3	ATP
3895	N-BUTANOL	181	10	0.15		C10H16N5O13P3	ATP
3896	PRIM. PENTANOLS	181	10	1.04		C10H16N5O13P3	ATP
3897	HEXANOL	181	18	1.18		C10H16N5O13P3	ATP
3898	OCTANOL	218		2.14	2.14 =	C10H16O1	ADAMANTANE,1-HYDROXY
3899	DIETHYL ETHER	212		1.45	1.38 A	C10H16O4	CAMPHORIC ACID
3900	CHCL3	46		-1.30	0.04 A	C10H16O4	CAMPHORIC ACID

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
3901	XYLENE	46		-1.81	-0.18 A	C10H16O4	CAMPHORIC ACID
3902	OCTANOL	348		0.75	0.75 =	C10H17N1O2	N-PENTANOYLCYCLOBUTANECARBOXAMIDE
3903	OCTANOL	348		0.48	0.48 =	C10H17N1O2	N-I-PENTANOYLCYCLOBUTANECARBOXAMIDE
3904	OCTANOL	348		0.53	0.53 =	C10H17N1O2	N-T-PENTANOYLCYCLOBUTANECARBOXAMIDE
3905	OCTANOL	134		0.49	0.49 =	C10H17N5O2	3-MORPHOLINO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
3906	OCTANOL	227		3.30	3.30 =	C10H18CL1N2O2	1-(2-CLET)-3(4-MECYCLOHEXYL)-1-NITROSOUREA (95441)
3907	CHCL3	424	46	-3.67		C10H18I1N1O2	QUINUCLIDINOL-3-ACETATE METHIODIDE
3908	CHCL3	67		-2.90		C10H18N2O4	O,L,-LYSINE,DIACETYL
3909	OCTANOL	134		3.21	3.21 =	C10H18N4O1S1	3-N-BUTYLTHIO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
3910	OCTANOL	134		2.68	2.68 =	C10H18N4O1S1	3-METHIO-4-AMINO-6-N-HEXYL-1,2,4-TRIAZINE-5-ONE
3911	DIETHYL ETHER	212		1.76	1.65 A	C10H18O4	SEBACIC ACID
3912	CHCL3	194		0.04	1.40 A	C10H18O4	SEBACIC ACID
3913	DIETHYL ETHER	2		-0.28	-0.13 A	C10H18O6	TRIETHYLENE GLYCOL DIACETATE
3914	OILS	2		-1.48	-0.79 B	C10H18O6	TRIETHYLENE GLYCOL,DIACETATE
3915	OILS	2		-1.48	-0.11 A	C10H18O6	TRIETHYLENE GLYCOL,DIACETATE
3916	OILS	290		0.52	1.66 A	C10H19N1O3	ETHYLPROPYLACETURETHANE/EPRONAL/
3917	OCTANOL	134		1.78	1.78 =	C10H19N5O1	3-N-BUTYLAMINO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
3918	PARAFFINS	241		0.52		C10H20N2S1	N-HEPTYLETHYLENETHIOUREA
3919	DIETHYL ETHER	378	44	-1.20	-0.11 B	C10H20N2O2	N-ALLYLCARBAMIC ACID,DIETAMINOETHYL ESTER
3920	OILS	173		2.27	3.25 A	C10H20O1	MENTHOL
3921	OILS	224		2.40	3.37 A	C10H20O1	MENTHOL
3922	OCTANOL	218		4.09	4.09 =	C10H20O2	DECANOIC ACID
3923	N-HEPTANE	139	31	1.87		C10H20O2	DECANOIC ACID
3924	OCTANOL	438		1.18	1.18 =	C10H20O6	GLUCOPYRANOSIDE,4-T-BUTYL (BETA)
3925	CHCL3	425		0.20	0.77 N	C10H20O6	GLUCOSE,2,3,4,6-TETRAMETHYL
3926	CHCL3	425		0.52	1.08 N	C10H20O6	B-METHYLGLUCOSIDE,2,3,4-TRIMETHYL
3927	CHCL3	396	31	3.37	2.65 B	C10H21N1	PROPYLHEXEDRINE
3928	N-HEPTANE	396	31	2.24		C10H21N1	PROPYLHEXEDRINE
3929	DIETHYL ETHER	378	44	-0.46	0.54 B	C10H22N2O2	N-PROPYLCARBAMIC ACID,DIETAMINOETHYL ESTER
3930	DIETHYL ETHER	378	44	-0.50	0.50 B	C10H22N2O2	N-I-PROPYLCARBAMIC ACID,DIETAMINOETHYL ESTER
3931	DIETHYL ETHER	3		1.32	1.27 A	C10H22O2	DECAMETHYLENEGLYCOL
3932	OILS	2		-2.25	-1.42 B	C10H22O5	TETRAETHYLENEGLYCOL,DIMETHYL ETHER
3933	DI-BUTYL ETHER	236	17	0.79		C10H23O4P1	DI-AMYLPHOSPHATE
3934	OCTANOL	298		4.02	4.02 =	C10H24SI1	SILANE, OCTYL-DIMETHYL
3935	CYCLOHEXANE	141		2.49		C11H6CL2O2	1,4-NAPHTHOQUINONE,2,3-DICHLORO,5-METHYL
3936	CYCLOHEXANE	141		3.06		C11H6CL2O2	1,4-NAPHTHOQUINONE,2,3-DICHLORO,6-METHYL
3937	CYCLOHEXANE	141		2.85		C11H7BR1O2	1,4-NAPHTHOQUINONE,2-METHYL,3-BROMO
3938	CYCLOHEXANE	141		2.17		C11H7BR1O3	1,4-NAPHTHOQUINONE,2-BROMO,3-METHOXY
3939	CYCLOHEXANE	141		2.61		C11H7CL1O2	1,4-NAPHTHOQUINONE,2-METHYL,3-CHLORO
3940	CHCL3	407	14	1.45		C11H8CL1N1O2	5-CHLORO-8-ACETOXYQUINOLINE
3941	CYCLOHEXANE	141		1.56		C11H8N2	MALONONITRILE, A-METHYLBENZAL
3942	CYCLOHEXANE	304		1.85		C11H8N2	MALONONITRILE,2-METHYLBENZAL
3943	CYCLOHEXANE	304		2.04		C11H8N2	MALONONITRILE,4-METHYLBENZAL
3944	CYCLOHEXANE	304		2.11		C11H8N2	MALONONITRILE,3-METHYLBENZAL
3945	CYCLOHEXANE	304		1.46		C11H8N2O1	MALONONITRILE,4-METHOXYBENZAL
3946	CYCLOHEXANE	304		1.68		C11H8N2O1	MALONONITRILE,3-METHOXYBENZAL
3947	CYCLOHEXANE	304		1.94		C11H8N2O1	MALONONITRILE,2-METHOXYBENZAL
3948	CYCLOHEXANE	141		0.30		C11H8N2O2	MALONONITRILE,3-METHOXY-4-HYDROXYBENZAL
3949	OCTANOL	141		2.10	2.10 =	C11H8O2	1,4-NAPHTHOQUINONE, 6-METHYL
3950	OCTANOL	141		2.20	2.20 =	C11H8O2	1,4-NAPHTHOQUINONE, 2-METHYL
3951	CYCLOHEXANE	141		1.82		C11H8O2	1,4-NAPHTHOQUINONE,6-METHYL
3952	CYCLOHEXANE	141		1.84		C11H8O2	1,4-NAPHTHOQUINONE,5-METHYL
3953	CYCLOHEXANE	141		1.88		C11H8O2	1,4-NAPHTHOQUINONE,2-METHYL
3954	CYCLOHEXANE	141		1.87		C11H8O2S1	1,4-NAPHTHOQUINONE,2-METHYLTHIO
3955	CHCL3	388		3.17	4.10 A	C11H8O2S1SE1	1-(2-SELENOPHEN-YL)-3(2-THIENYL)-1,3-PROPANEDIONE
3956	BENZENE	388		2.75	4.07 A	C11H8O2S1SE1	1-(2-SELENOPHEN-YL)-3(2-THIENYL)-1,3-PROPANEDIONE
3957	CHCL3	388		3.17	4.10 A	C11H8O2SE2	1,3-DI(2-SELENOPHEN-YL)-1,3-PROPANEDIONE
3958	BENZENE	388		3.16	4.46 A	C11H8O2SE2	1,3-DI(2-SELENOPHEN-YL)-1,3-PROPANEDIONE
3959	CYCLOHEXANE	304		0.66		C11H8O3	COUMARIN,3-ACETYL
3960	OCTANOL	141	26	1.35	1.35 =	C11H8O3	1,4-NAPHTHOQUINONE, 2-METHOXY
3961	CYCLOHEXANE	141		0.48		C11H8O3	1,4-NAPHTHOQUINONE,2-METHOXY
3962	OCTANOL	141		1.20	1.20 =	C11H8O3	1,4-NAPHTHOQUINONE,2-METHYL-3-HYDROXY
3963	CYCLOHEXANE	141		0.79		C11H8O3	1,4-NAPHTHOQUINONE,2-METHYL,3-HYDROXY
3964	CHCL3	388		3.10	4.03 A	C11H8O3SE1	1-(2-SELENOPHEN-YL)-3(2-FURYL)-1,3-PROPANEDIONE
3965	BENZENE	388		2.68	4.00 A	C11H8O3SE1	1-(2-SELENOPHEN-YL)-3(2-FURYL)-1,3-PROPANEDIONE
3966	OCTANOL	65		2.45	2.45 =	C11H9N1	4-PHENYLPYRIDINE
3967	OCTANOL	216		1.58	1.58 =	C11H9N1O1	6-ACETYLQUINOLINE
3968	PARAFFINS	439		-0.33		C11H10N2	2-(P-AMINOPHENYL)-PYRIDINE
3969	CYCLOHEXANE	304		-0.73		C11H10N2O1	CYANOACETAMIDE,2-METHYLBENZAL
3970	CYCLOHEXANE	304		-0.54		C11H10N2O1	CYANOACETAMIDE,4-METHYLBENZAL
3971	CYCLOHEXANE	304		-1.10		C11H10N2O2	CYANOACETAMIDE,4-METHOXYBENZAL
3972	CYCLOHEXANE	304		-0.92		C11H10N2O2	CYANOACETAMIDE,2-METHOXYBENZAL
3973	CYCLOHEXANE	304		-0.91		C11H10N2O2	CYANOACETAMIDE,3-METHOXYBENZAL
3974	CYCLOHEXANE	280		2.02		C11H11N1	2,6-DIMETHYLQUINOLINE
3975	CYCLOHEXANE	141		2.65		C11H11N1O4	STYRENE,3,4-DIOXYMETHYLENE,B-NITRO,B-ETHYL
3976	CYCLOHEXANE	141		2.30		C11H11N1O4	STYRENE,4-METHOXYCARBONYL,B-NITRO,B-METHYL
3977	OCTANOL	235		2.28	2.28 =	C11H11N3O1	1-PHENYL-3,5-DIMETHYL-4-NITROSOPYRAZOLE
3978	OILS	284		0.83	1.94 A	C11H11N3O1	1-PHENYL-3,5-DIMETHYL-4-NITROSOPYRAZOLE
3979	OCTANOL	393	63	-0.02	-0.02 =	C11H11N3O2S1	SULFAPYRIDINE
3980	OCTANOL	56		0.00	0.00 =	C11H11N3O2S1	SULFAPYRIDINE
3981	DIETHYL ETHER	342		-0.40	-0.23 A	C11H11N3O2S1	SULFAPYRIDINE
3982	DIETHYL ETHER	113		-0.26	-0.12 A	C11H11N3O2S1	SULFAPYRIDINE
3983	CHCL3	343	2	0.02	-0.21 B	C11H11N3O2S1	SULFAPYRIDINE
3984	CHCL3	113		0.06	-0.18 B	C11H11N3O2S1	SULFAPYRIDINE
3985	CHCL3	393	63	0.04	-0.20 B	C11H11N3O2S1	SULFAPYRIDINE
3986	BENZENE	343	2	-0.75	0.03 B	C11H11N3O2S1	SULFAPYRIDINE
3987	1-PENT. ACETATE	343	2	0.35	0.19	C11H11N3O2S1	SULFAPYRIDINE
3988	CCL4	343	2	-2.22	0.00 A	C11H11N3O2S1	SULFAPYRIDINE
3989	OCTANOL	65	46	-2.76	-2.76 =	C11H12BR1N1	ETHYLQUINOLINIUM BROMIDE
3990	OCTANOL	9		1.14	1.14 =	C11H12CL2N2O5	CHLORAMPHENICOL
3991	DIETHYL ETHER	440	12	0.62	0.67 A	C11H12CL2N2O5	CHLORAMPHENICOL
3992	CHCL3	440	12	-0.65	0.64 A	C11H12CL2N2O5	CHLORAMPHENICOL
3993	BENZENE	440	12	-1.45	0.00 A	C11H12CL2N2O5	CHLORAMPHENICOL
3994	ETHYL ACETATE	440		1.52	1.57	C11H12CL2N2O5	CHLORAMPHENICOL
3995	PARAFFINS	440		-1.48		C11H12CL2N2O5	CHLORAMPHENICOL
3996	OLEYL ALCOHOL	406		2.93	3.50	C11H12CL3N1O2S1	N-TRICLMETHIO-4,5-DIMETHYLTETRAHYDROPHTHALIMIDE
3997	CHCL3	306		1.70	2.69 A	C11H12I1N1O4S1	N-(P-IODOBENZENESULFONYL)PROLINE
3998	CCL4	306		-0.18	1.69 A	C11H12I1N1O4S1	N-(P-IODOBENZENESULFONYL)PROLINE
3999	CLCH2CH2CL	306		1.70		C11H12I1N1O4S1	N-(P-IODOBENZENESULFONYL)PROLINE
4000	DIETHYL ETHER	306		0.67	0.66 A	C11H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)HYDROXYPROLINE

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4001	CHCL3	306		-0.72	0.55 A	C11H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)HYDROXYPROLINE
4002	ETHYL ACETATE	306	12	1.65	1.78 A	C11H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)HYDROXYPROLINE
4003	CCL4	306		-2.00	0.15 A	C11H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)HYDROXYPROLINE
4004	CLCH2CH2CL	306		-0.25		C11H12I1N1O5S1	N-(P-IODOBENZENESULFONYL)HYDROXYPROLINE
4005	DIETHYL ETHER	306		1.23	1.25 A	C11H12I1N1O6S1	N-(P-IODOBENZENESULFONYL)GLUTAMIC ACID
4006	CHCL3	306	12	-2.00	-0.58 A	C11H12I1N1O6S1	N-(P-IODOBENZENESULFONYL)GLUTAMIC ACID
4007	CLCH2CH2CL	306		-1.15		C11H12I1N1O6S1	N-(P-IODOBENZENESULFONYL)GLUTAMIC ACID
4008	OILS	382	24	4.99	5.72 A	C11H12I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,BUTYL ESTER
4009	OILS	382	24	5.01	5.75 A	C11H12I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,S-BUTYL ESTER
4010	OILS	382	24	2.35	3.33 A	C11H12I2O4	BENZOIC ACID,4-OH,3,5-DI-IODO,O-OH-BUTYL ESTER
4011	N-HEPTANE	441	12	-4.52		C11H12N2	TETRAHYDRO-B-CARBOLINE
4012	OCTANOL	186		0.23	0.23 =	C11H12N2O1	ANTIPYRINE
4013	DIETHYL ETHER	3		-1.14	-0.16 B	C11H12N2O1	ANTIPYRINE
4014	CHCL3	394		0.88	0.53 B	C11H12N2O1	ANTIPYRINE
4015	CHCL3	344	12	1.45	1.00 B	C11H12N2O1	ANTIPYRINE
4016	CHCL3	254	12	1.33	0.91 B	C11H12N2O1	ANTIPYRINE
4017	CHCL3	338	44	1.45	1.01 B	C11H12N2O1	ANTIPYRINE
4018	OILS	2		-1.49	-0.12 A	C11H12N2O1	ANTIPYRINE
4019	OILS	69		-1.16	0.15 A	C11H12N2O1	ANTIPYRINE
4020	BENZENE	338	44	-1.05		C11H12N2O1	ANTIPYRINE
4021	1-BUTANOL	4		0.51	0.21	C11H12N2O1	ANTIPYRINE
4022	N-HEPTANE	254		-2.30		C11H12N2O1	ANTIPYRINE
4023	N-HEPTANE	338	44	-1.40		C11H12N2O1	ANTIPYRINE
4024	N-HEPTANE	340		-2.30		C11H12N2O1	ANTIPYRINE
4025	OLEYL ALCOHOL	82		-0.52	0.05	C11H12N2O1	ANTIPYRINE
4026	OCTANOL	218		1.53	1.53 =	C11H12N2O2	HYDANTOIN,5-ETHYL-5-PHENYL
4027	CYCLOHEXANE	304		-2.86		C11H12N2O2	MALONAMIDE,2-METHYLBENZAL
4028	CYCLOHEXANE	304		-2.80		C11H12N2O2	MALONAMIDE,4-METHYLBENZAL
4029	CYCLOHEXANE	304		-2.68		C11H12N2O2	MALONAMIDE,3-METHYLBENZAL
4030	OCTANOL	56		-1.04	-1.04 =	C11H12N2O2	TRYPTOPHAN, DL
4031	CYCLOHEXANE	304		-4.00		C11H12N2O3	MALONAMIDE,2-METHOXYBENZAL
4032	CYCLOHEXANE	304		-3.52		C11H12N2O3	MALONAMIDE,4-METHOXYBENZAL
4033	CYCLOHEXANE	304		-3.42		C11H12N2O3	MALONAMIDE,3-METHOXYBENZAL
4034	OCTANOL	393	63	0.13	0.13 =	C11H12N4O2S1	SULFAMERAZINE
4035	OCTANOL	56		0.14	0.14 =	C11H12N4O2S1	SULFAMERAZINE
4036	DIETHYL ETHER	113	15	-0.18	-0.05 A	C11H12N4O2S1	SULFAMERAZINE
4037	CHCL3	343	2	0.38	0.09 B	C11H12N4O2S1	SULFAMERAZINE
4038	CHCL3	113	15	0.45	0.15 B	C11H12N4O2S1	SULFAMERAZINE
4039	CHCL3	393	63	0.48	0.18 B	C11H12N4O2S1	SULFAMERAZINE
4040	BENZENE	343	2	-0.69	0.07 B	C11H12N4O2S1	SULFAMERAZINE
4041	1-PENT. ACETATE	343	2	0.32	0.16	C11H12N4O2S1	SULFAMERAZINE
4042	CCL4	343	2	-1.66	0.46 A	C11H12N4O2S1	SULFAMERAZINE
4043	1-BUTANOL	130	13	0.32	-0.06	C11H12N4O3S	SULFAMETHOXYPYRIDAZINE
4044	1-BUTANOL	130	13	0.85	0.69	C11H12N4O3S	SULFAMETHOXYPYRIDAZINE
4045	OCTANOL	393	63	0.40	0.40 =	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4046	CHCL3	343	2	0.62	1.17 N	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4047	CHCL3	344	44	0.90	1.38 N	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4048	CHCL3	393	63	0.67	0.34 B	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4049	BENZENE	343	2	-0.57	0.82 A	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4050	1-PENT. ACETATE	343	2	0.12	-0.05	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4051	CCL4	343	2	-2.52	-0.25 A	C11H12N4O3S1	SULFAMETHOXYPYRIDAZINE
4052	OCTANOL	393	63	0.85	0.85 =	C11H12N4O3S1	SULFAMONOMETHOXINE
4053	CHCL3	343	2	0.63	1.18 N	C11H12N4O3S1	SULFAMONOMETHOXINE
4054	CHCL3	393	63	0.71	1.26 N	C11H12N4O3S1	SULFAMONOMETHOXINE
4055	BENZENE	343	2	-0.10	1.31 A	C11H12N4O3S1	SULFAMONOMETHOXINE
4056	1-BUTANOL	130	13	0.60	0.34	C11H12N4O3S1	SULFAMONOMETHOXINE
4057	1-PENT. ACETATE	343	2	1.17	1.03	C11H12N4O3S1	SULFAMONOMETHOXINE
4058	CCL4	343	2	-0.70	1.25 A	C11H12N4O3S1	SULFAMONOMETHOXINE
4059	CYCLOHEXANE	304		3.27		C11H12O2	CINNAMIC ACID,ETHYL ESTER
4060	OCTANOL	10		2.33	2.33 =	C11H12O3	5-INDANOXYACETIC ACID
4061	N-BUTANOL	295	52	0.30	-0.08	C11H13CL1N2O2	TRYPTOPHANE HYDROCHLORIDE
4062	CYCLOHEXANE	141		3.82		C11H13N1O2	STYRENE,4-I-PROPYL,B-NITRO
4063	CYCLOHEXANE	141		3.10		C11H13N1O2	STYRENE,4-METHYL,B-NITRO,B-ETHYL
4064	CYCLOHEXANE	141		3.61		C11H13N1O2	STYRENE,2-METHYL,B-NITRO,B-ETHYL
4065	CHCL3	67		-0.70		C11H13N1O3	L-PHENYLALANINE,ACETYL
4066	CYCLOHEXANE	141		3.07		C11H13N1O3	STYRENE,2-ETHOXY,B-NITRO,B-METHYL
4067	CYCLOHEXANE	141		2.49		C11H13N1O3	STYRENE,4-METHOXY,B-NITRO,B-ETHYL
4068	CYCLOHEXANE	141		2.88		C11H13N1O3	STYRENE,2-METHOXY,B-NITRO,B-ETHYL
4069	CYCLOHEXANE	141		2.88		C11H13N1O3	STYRENE,3-METHOXY,B-NITRO,B-ETHYL
4070	CHCL3	67		-2.78		C11H13N1O4	N-ACETYLTYROSINE/L/
4071	ETHYL ACETATE	67		-0.15	-0.21	C11H13N1O4	N-ACETYLTYROSINE/L/
4072	DIETHYL ETHER	431		-0.66	-0.43 A	C11H13N1O4	BENZOYLTHREONINE
4073	CYCLOHEXANE	141		1.71		C11H13N1O4	STYRENE,3,4-DIMETHOXY,B-NITRO,B-METHYL
4074	CYCLOHEXANE	141		2.49		C11H13N1O4	STYRENE,2,5-DIMETHOXY,B-NITRO,B-METHYL
4075	CYCLOHEXANE	141		2.54		C11H13N1O4	STYRENE,2,4-DIMETHOXY,B-NITRO,B-METHYL
4076	CYCLOHEXANE	141		2.57		C11H13N1O4	STYRENE,2,3-DIMETHOXY,B-NITRO,B-METHYL
4077	CYCLOHEXANE	141		1.49		C11H13N1O4	STYRENE,4-HYDROXY,3-ETHOXY,B-NITRO,B-METHYL
4078	CYCLOHEXANE	141		1.57		C11H13N1O4	STYRENE,4-HYDROXY,3-METHOXY,B-NITRO,B-ETHYL
4079	CHCL3	338	44	1.17	0.77 B	C11H13N3O1	4-AMINOANTIPYRINE
4080	BENZENE	338	44	-0.92		C11H13N3O1	4-AMINOANTIPYRINE
4081	N-HEPTANE	338	44	-1.52		C11H13N3O1	4-AMINOANTIPYRINE
4082	OCTANOL	393	63	1.15	1.15 =	C11H13N3O3S1	SULFISOXAZOLE
4083•	OCTANOL	56		1.01	1.01 =	C11H13N3O3S1	SULFISOXAZOLE
4084	CHCL3	343	2	0.64	1.19 N	C11H13N3O3S1	SULFISOXAZOLE
4085	CHCL3	393	63	0.94	1.35 N	C11H13N3O3S1	SULFISOXAZOLE
4086	CHCL3	415	44	0.07	0.67 N	C11H13N3O3S1	SULFISOXAZOLE
4087	BENZENE	343	2	-0.07	1.34 A	C11H13N3O3S1	SULFISOXAZOLE
4088	1-PENT. ACETATE	343	2	1.35	1.22	C11H13N3O3S1	SULFISOXAZOLE
4089	CCL4	343	2	-1.48	0.61 A	C11H13N3O3S1	SULFISOXAZOLE
4090	N-HEPTANE	415	44	-3.57		C11H13N3O3S1	SULFISOXAZOLE
•4091	N-HEPTANE	416	14	0.98		C11H14CL1N1O3	P-AMINOSALICYLIC ACID,4-CHLOROBUTYL ESTER
4092	N-HEPTANE	138		1.78		C11H14F3N1	N-METHYLNORFENFLURAMINE
4093	CHCL3	306		1.38	2.41 A	C11H14I1N1O4S1	N-(P-IODOBENZENESULFONYL)VALINE
4094	CCL4	306		-0.32	1.57 A	C11H14I1N1O4S1	N-(P-IODOBENZENESULFONYL)VALINE
4095	CLCH2CH2CL	306		1.60		C11H14I1N1O4S1	N-(P-IODOBENZENESULFONYL)VALINE
4096	CHCL3	306	12	1.38	2.41 A	C11H14I1N1O4S2	N-(P-IODOBENZENESULFONYL)METHIONINE
4097	CCL4	306		-0.58	1.35 A	C11H14I1N1O4S2	N-(P-IODOBENZENESULFONYL)METHIONINE
4098	CLCH2CH2CL	306		1.30		C11H14I1N1O4S2	N-(P-IODOBENZENESULFONYL)METHIONINE
4099	OCTANOL	430	46	-0.69	-0.69 =	C11H14N2.H3PO4	5-METHYLTRYPTAMINE PHOSPHATE
4100	OCTANOL	430	46	-1.57	-1.57 =	C11H14N2O1.H3PO4	5-METHOXYTRYPTAMINE PHOSPHATE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4101	CYCLOHEXANE	141		2.56		C11H14N2O2	STYRENE,4-DIMETHYLAMINO,B-NITRO,B-METHYL
4102	CHCL3	399	1	2.15	1.62 B	C11H14N2O3	ALLOBARBITAL,N-METHYL
4103	I-PENT. ACETATE	399	1	1.93	1.82	C11H14N2O3	ALLOBARBITAL,N-METHYL
4104	CCL4	399	1	0.84		C11H14N2O3	ALLOBARBITAL,N-METHYL
4105	MIXED SOLV#1	433		0.88		C11H14N2O3	ALLOBARBITAL,N-METHYL
4106	OCTANOL	428		-0.03	-0.03 =	C11H14N2O5	N-ACETYL-A-HYDROXYMETHYL-B-OH-4-NITROPHENETHYL AMINE
4107	OCTANOL	226		0.09	0.09 =	C11H14N4O4S1	6-METHYLTHIO-9-B-D-RIBOFURANOSYL-9-H-PURINE (40774)
4108	OCTANOL	255		2.42	2.42 =	C11H14O1	2-PENTANONE,5-PHENYL
4109	OCTANOL	255		2.77	2.77 =	C11H14O2	ACETIC ACID,G-PHENYLPROPYL ESTER
4110	OCTANOL	255		2.77	2.77 =	C11H14O2	4-PHENYLBUTYRIC ACID,METHYL ESTER
4111	OILS	362		0.84	1.98 A	C11H14O2	A-PHENYLVALERIC ACID
4112	OILS	385		1.41	2.47 A	C11H14O2	2-PHENYLVALERIC ACID
4113	OILS	417		1.46	2.52 A	C11H14O2	4-PHENYLVALERIC ACID
4114	OILS	361		1.03	2.19 A	C11H14O2	5-PHENYLVALERIC ACID
4115	OCTANOL	56		3.57	3.57 =	C11H14O3	P-HYDROXYBENZOIC ACID,BUTYL ESTER
4116	OCTANOL	10		2.59	2.59 =	C11H14O3	PHENOXYACETIC ACID,3-ISOPROPYL
4117	OCTANOL	10		2.69	2.69 =	C11H14O3	PHENOXYACETIC ACID,4-ISOPROPYL
4118	OCTANOL	10		2.71	2.71 =	C11H14O3	PHENOXYACETIC ACID,3-PROPYL
4119	OILS	345		0.63	1.76 A	C11H15BRN2O3	BARBITURIC ACID,S-BUTYL,B-BROMOALLYL
4120	OCTANOL	437		3.46	3.46 =	C11H15CL2O6P1S1	O,O-DIET-O-(2,6-CL2-4-MESULFONYLPHENYL)PHOSPHATE
4121	TOLUENE	150		3.28	4.45 A	C11H15N1O1	N-BUTYL-SALICYLIDENEIMINE (SCHIFF BASE)
4122	CHCL3	396	31	2.28	1.73 B	C11H15N1O1	PHENMETRAZINE
4123	N-HEPTANE	396	31	0.32		C11H15N1O1	PHENMETRAZINE
4124	OLEYL ALCOHOL	390	44	2.77	3.31	C11H15N1O2	P-AMINOBENZOIC ACID,BUTYL ESTER
4125	I-PENT. ACETATE	418	3	3.76	3.72	C11H15N1O2	P-AMINOBENZOIC ACID,I-BUTYL ESTER
4126	I-PENT. ACETATE	418	3	3.78	3.74	C11H15N1O2	P-AMINOBENZOIC ACID,N-BUTYL ESTER
4127	I-PENT. ACETATE	418	3	3.58	3.52	C11H15N1O2	P-AMINOBENZOIC ACID, SEC-BUTYL ESTER
4128	I-PENT. ACETATE	418	3	3.08	3.01	C11H15N1O2	P-AMINOBENZOIC ACID,T-BUTYL ESTER
4129	HEXANE	391		1.09		C11H15N1O2	N-METHYL CARBAMATE,3-I-PROPYLPHENYL
4130	HEXANE	391		0.89		C11H15N1O2	N-METHYL CARBAMATE,3,4,6-TRIMETHYLPHENYL
4131	HEXANE	391		0.93		C11H15N1O2	N-METHYL CARBAMATE,3,4,5-TRIMETHYLPHENYL
4132	OCTANOL	384		2.31	2.31 =	C11H15N1O2	N-METHYL-2-I-PROPYLPHENYLCARBAMATE
4133	OCTANOL	384		2.40	2.40 =	C11H15N1O2	N-METHYL-2-PROPYLPHENYLCARBAMATE
4134	OCTANOL	384		2.63	2.63 =	C11H15N1O2	N-METHYL-3-I-PROPYLPHENYLCARBAMATE
4135	OCTANOL	384		2.80	2.80 =	C11H15N1O2	N-METHYL-4-I-PROPYLPHENYLCARBAMATE
4136	OCTANOL	255		-0.36	-0.36 =	C11H15N1O2	VALERIC ACID,2-AMINO-5-PHENYL
4137	HEXANE	391		1.48		C11H15N1O2S1	N-METHYL CARBAMATE,3,5-DIMETHYL,4-METHYLTHIOPHENYL
4138	N-HEPTANE	370	14	1.17		C11H15N1O3	P-AMINOSALICYLIC ACID,N-BUTYL ESTER
4139	OCTANOL	384		1.52	1.52 =	C11H15N1O3	N-METHYL-2-I-PROPOXYPHENYLCARBAMATE
4140	HEXANE	376		-0.14		C11H15N1O3	N-METHYLCARBAMIC ACID,O-I-PROPOXYPHENYL ESTER
4141	N-HEPTANE	370	14	0.18		C11H15N1O4	P-AMINOSALICYLIC ACID,4-HYDROXYBUTYL ESTER
4142	CHCL3	322		-2.00	-1.25 N	C11H15N5O5	1-METHYLGUANOSINE
4143	N-HEPTANE	421	44	2.69		C11H16CL1N1	G-(P-CHLOROPHENYL)-PROPYLDIMETHYLAMINE
4144	OCTANOL	437		2.92	2.92 =	C11H16CL1O4P1S1	O,O-DIET-O-(3-CL-4-METHYLTHIOPHENYL)PHOSPHATE
4145	OCTANOL	349		2.20	2.20 =	C11H16N1O5P1	PHOSPHONATE,O-(P-NITROPHENYL)-O-PROPYL,ETHYL
4146	OCTANOL	437		2.01	2.01 =	C11H16N1O6P1S1	O,O-DIET-O-(2-NITRO-4-METHIOPHENYL)PHOSPHATE
4147	OCTANOL	341	60	1.68	1.68 =	C11H16N2	4-(N,N-DIMETHYL)-3-PYRIDYLBUTENE-1-YLAMINE
4148	OCTANOL	341	60	0.96	0.96 =	C11H16N2	METHYLANABASINE
4149	PARAFFINS	316		0.55		C11H16N2	4-(N-PIPERIDYL)-ANILINE
4150	OCTANOL	341	60	1.34	1.34 =	C11H16N2	3-PYRIDYLETHYL-2-(N-PYRROLIDINE)
4151	N-HEPTANE	419		-0.92		C11H16N2O1	UREA,ETHYL-M-PHENETYL/UNSYM/
4152	N-HEPTANE	419		-1.20		C11H16N2O1	UREA,ETHYL-O-PHENETYL/UNSYM/
4153	N-HEPTANE	419		-1.07		C11H16N2O1	UREA,ETHYL-P-PHENETYL/UNSYM/
4154	N-HEPTANE	419		-0.25		C11H16N2O1	UREA,N-BUTYLPHENYL-
4155	N-HEPTANE	419		-0.28		C11H16N2O1	UREA,N-PROPYL,M-TOLYL-
4156	N-HEPTANE	419		-0.49		C11H16N2O1	UREA,N-PROPYL,O-TOLYL-
4157	N-HEPTANE	419		-0.49		C11H16N2O1	UREA,N-PROPYL,P-TOLYL-
4158	HEXANE	391		0.12		C11H16N2O2	N-METHYL CARBAMATE,3-METHYL,4-DIMETHYLAMINOPHENYL
4159	N-HEPTANE	400	14	-3.25		C11H16N2O2	PILOCARPINE
4160	50%ETHER+50%DMF	125		0.82	2.84	C11H16N2O2S1	5-ALLYL-5-I-BUTYL-2-THIOBARBITURIC ACID/BUTHALITAL/
4161	50%ETHER+50%DMF	125		0.52	2.10	C11H16N2O3	5-ALLYL-5-BUTYLBARBITURIC ACID
4162	50%ETHER+50%DMF	125		0.61	2.32	C11H16N2O3	5-ALLYL-5-I-PR-1-METHYLBARBITURIC ACID
4163	OILS	345		0.39	1.55 A	C11H16N2O3	BARBITURIC ACID,ALLYL,S-BUTYL
4164	HEXANE	372		1.02		C11H16O1	PENTANOL,5-PHENYL
4165	CHCL3	396	31	3.46	2.74 B	C11H17N1	DIMETHYLAMPHETAMINE
4166	N-HEPTANE	396	31	2.03		C11H17N1	DIMETHYLAMPHETAMINE
4167	DIETHYL ETHER	374		1.80	2.44 B	C11H17N1	N-ETHYL-G-PHENYLPROPYLAMINE
4168	CHCL3	396	31	3.25	2.56 B	C11H17N1	ETHYLAMPHETAMINE
4169	N-HEPTANE	138		1.88		C11H17N1	ETHYLAMPHETAMINE
4170	N-HEPTANE	396	31	1.59		C11H17N1	ETHYLAMPHETAMINE
4171	CHCL3	396	31	2.94	2.29 B	C11H17N1	MEPHENTERMINE
4172	N-HEPTANE	396	31	2.04		C11H17N1	MEPHENTERMINE
4173	OCTANOL	255		2.73	2.73 =	C11H17N1	G-PHENYLPROPYLDIMETHYLAMINE
4174	N-HEPTANE	421	44	2.03		C11H17N1	G-PHENYLPROPYLDIMETHYLAMINE
4175	XYLENE	422		1.81	2.47 B	C11H17N1	PROPYL AMINE,N-ME,N-(1-BENZYL)
4176	OCTANOL	302		2.29	2.29 =	C11H17N1O1	P-DIETHYLAMINOBENZYL ALCOHOL
4177	CHCL3	396	31	1.91	1.41 B	C11H17N1O1	METHYLEPHEDRINE
4178	N-HEPTANE	396	31	-0.04		C11H17N1O1	METHYLEPHEDRINE
4179	OCTANOL	397		1.16	1.16 =	C11H17N5O1	ADENINE,9-(I-HYDROXYMETHYL-PENTYL)
4180	OCTANOL	437		2.24	2.24 =	C11H17O4P1S1	O,O-DIETHYL-O-(4-METHYLTHIOPHENYL)PHOSPHATE
4181	OCTANOL	437		0.00	0.00 =	C11H17O6P1S1	O,O-DIETHYL-O-(4-METHYLSULFONYLPHENYL)PHOSPHATE
4182	OCTANOL	65	46	-3.38	-3.38 =	C11H18BR1N1	BENZYLDIMETHYLETHYLAMMONIUM BROMIDE
4183	OCTANOL	65	53	-2.03	-2.03 =	C11H18BR1N1	HEXYLPYRIDINIUM BROMIDE
4184	OCTANOL	341	60	1.23	1.23 =	C11H18N2	N,N-DIETHYL-3-PYRIDYLETHYLAMINE
4185	OCTANOL	341	60	1.49	1.49 =	C11H18N2	4-(N,N-DIMETHYL)-3-PYRIDYLBUTYLAMINE
4186	N-HEPTANE	400	14	-2.48		C11H18N2O2.HBR	SPIRO-(N'-METHYLPIPERIDYL-4')-N-ETSUCCINIMIDE
4187	OCTANOL	218		2.98	2.98 =	C11H18N2O2S1	BARBITURIC ACID,5-ETHYL-5-I-AMYL-2-THIO
4188	CHCL3	399	1	2.51	2.95 N	C11H18N2O2S1	BARBITURIC ACID,5-ETHYL-5-I-AMYL-2-THIO
4189	I-PENT. ACETATE	399	1	3.00	2.94	C11H18N2O2S1	BARBITURIC ACID,5-ETHYL-5-I-AMYL-2-THIO
4190	CCL4	399	1	1.58	3.21 A	C11H18N2O2S1	BARBITURIC ACID,5-ETHYL-5-I-AMYL-2-THIO
4191	CHCL3	338	44	2.22	2.69 N	C11H18N2O2S1	BARBITURIC ACID,ET,1-MEBU,2-THIO/THIOPENTAL/
4192	OILS	442		1.95	2.96 A	C11H18N2O2S1	BARBITURIC ACID,ET,1-MEBU,2-THIO/THIOPENTAL/
4193	OILS	398	44	1.80	2.83 A	C11H18N2O2S1	BARBITURIC ACID,ET,1-MEBU,2-THIO/THIOPENTAL/
4194	BENZENE	338	44	0.51		C11H18N2O2S1	BARBITURIC ACID,ET,1-MEBU,2-THIO/THIOPENTAL/
4195	N-HEPTANE	254		0.52		C11H18N2O2S1	BARBITURIC ACID,ET-1-MEBU,2-THIO/THIOPENTAL/
4196	N-HEPTANE	338	44	0.19		C11H18N2O2S1	BARBITURIC ACID,ET,1-MEBU,2-THIO/THIOPENTAL/
4197	N-HEPTANE	340		0.52		C11H18N2O2S1	BARBITURIC ACID,ET,1-MEBU,2-THIO/THIOPENTAL/
4198	OCTANOL	218		2.24	2.24 =	C11H18N2O3	BARBITURIC ACID,5-AMYL-5-ETHYL
4199	OILS	345		0.46	1.61 A	C11H18N2O3	BARBITURIC ACID,5-AMYL-5-ETHYL
4200	OCTANOL	399		2.07	2.07 =	C11H18N2O3	BARBITURIC ACID,5-ETHYL-5-I-AMYL/AMOBARBITAL/

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4201	CHCL3	399	1	1.73	2.24 N	C11H18N2O3	BARBITURIC ACIO,5-ETHYL-5-1-AMYL/AMOBARBITAL/
4202	OILS	345		0.46	1.61 A	C11H18N2O3	BARBITURIC ACIO,5-ETHYL-5-1-AMYL/AMOBARBITAL/
4203	BENZENE	399	1	0.72	2.10 A	C11H18N2O3	BARBITURIC ACIO,5-ETHYL-5-1-AMYL/AMOBARBITAL/
4204	1-PENT. ACETATE	399	1	2.13	2.03	C11H18N2O3	BARBITURIC ACIO,5-ETHYL-5-1-AMYL/AMOBARBITAL/
4205	CCL4	399	1	0.34	2.22 A	C11H18N2O3	BARBITURIC ACIO,5-ETHYL-5-I-AMYL/AMOBARBITAL/
4206	OCTANOL	399		2.03	2.03 =	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL
4207	CHCL3	399	1	1.38	1.90 N	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4208	OILS	345		0.64	1.77 A	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4209	OILS	398	44	0.76	1.88 A	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-ME BU)/PENTOBARBITAL/
4210	BENZENE	399	1	0.51	1.90 A	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4211	1-PENT. ACETATE	399	1	2.03	1.93	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4212	CCL4	399	1	-0.03	1.80 A	C11H18N2O3	BARBITURIC ACID,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4213	N-HEPTANE	340		-1.30		C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4214	50%ETHER+50%DMF	125		0.53	2.12	C11H18N2O3	BARBITURIC ACIO,5-ET-5-(1-MEBU)/PENTOBARBITAL/
4215	OCTANOL	218		0.35	0.35 =	C11H18N2O4	BARBITURIC ACIO, 5-ETHYL-5(3OH-1-METHYLBUTYL)
4216	OCTANOL	348		0.89	0.89 =	C11H19N1O2	N-HEXANOYLCYCLOBUTANECARBOXAMIOE
4217	CHCL3	424	46	-3.20		C11H20I1N1O2	N-METHYL-1-QUINUCLIDINOL-3-ACETATE METHIODIOE
4218	CHCL3	424	46	-3.71		C11H20I1N1O2	TROPINYL ACETATE-METHIODIDE/TRANS/
4219	CHCL3	424	46	-3.09		C11H20I1N1O2	TROPINYL ACETATE-METHIODIDE/CIS/
4220	SEC-BUTANOL	84	19	-1.31	-2.34	C11H21N5O5	ARGINYLGLUTAMIC ACIO
4221	CHCL3	424	46	-3.28		C11H22I1N1O2	1,2,6-TRIMETHYL-4-ACETYL PIPERIOINE METHIODIOE
4222	CHCL3	424	46	-3.09		C11H22I1N1O2	1,3,5-TRIMETHYL-4-ACETYL PIPERIOINE METHIODIOE
4223	DIETHYL ETHER	378	44	-1.06	-0.01 B	C11H22N2O3	MORPHOLINOFORMIC ACIO,DIETAMINOETHYL ESTER
4224	PARAFFINS	241		1.08		C11H22N2S1	N-OCTYLETHYLENETHIOUREA
4225	CHCL3	424	46	-2.70		C11H24I1N1	1,2,2,6,6-PENTAMETHYLPIPERIDINE METHIODIOE
4226	CHCL3	424	46	-2.52		C11H24I1N1	1,3,3,5,5-PENTAMETHYLPIPERIDINE METHIODIOE
4227	DIETHYL ETHER	378	44	-0.12	0.83 B	C11H24N2O2	N-BUTYLCARBAMIC ACIO,DIETAMINOETHYL ESTER
4228	DIETHYL ETHER	378	44	-1.02	0.04 B	C11H24N2O2	N-T-BUTYLCARBAMIC ACIO,DIETAMINOETHYL ESTER
4229	DIETHYL ETHER	378	44	-0.73	0.30 B	C11H24N2O2	N,N-DIETHYLCARBAMIC ACIO,DIETAMINOETHYL ESTER
4230	DIETHYL ETHER	378	44	-1.07	0.00 B	C11H24N2O2	N-SEC-BUTYLCARBAMIC ACIO,DIETAMINOETHYL ESTER
4231	OCTANOL	235		1.68	1.68 =	C11H24O2SN1	TRIPROPYLTIN ACETATE
4232	OCTANOL	297	46	-1.07	-1.07 =	C11H26I1N1	TRIMETHYL-OCTYL-AMMONIUM IODIDE
4233	OCTANOL	297	46	-2.19	-2.19 =	C11H26I1N1	TRIPROPYL-ETHYL-AMMONIUM IODIDE
4234	OCTANOL	298		4.24	4.24 =	C11H26S11	SILANE, OCTYL-TRIMETHYL
4235	CYCLOHEXANE	304		1.96		C12H6F2N2	MALONONITRILE,2,6-DIFLUOROCINNAMAL
4236	CYCLOHEXANE	304		1.96		C12H7CL1N2	MALONONITRILE,2-CHLOROCINNAMAL
4237	N-HEPTANE	443		0.81		C12H7CL2N1S1	PHENOTHIAZINE,2,7-DICHLORO
4238	N-HEPTANE	443		0.83		C12H7CL2N1S1	PHENOTHIAZINE,3,7-DICHLORO
4239	CYCLOHEXANE	304		1.80		C12H7F1N2	MALONONITRILE,2-FLUOROCINNAMAL
4240	CYCLOHEXANE	304		1.01		C12H7N3O2	MALONONITRILE,2-NITROCINNAMAL
4241	N-HEPTANE	443		3.60		C12H8BR1N1S1	PHENOTHIAZINE,3-BROMO
4242	N-HEPTANE	443		3.32		C12H8CL1N1S1	PHENOTHIAZINE,3-CHLORO
4243	HEXANE	317		5.00		C12H8CL6	ALORIN
4244	HEXANE	317		4.56		C12H8CL6O1	DIELORIN
4245	N-HEPTANE	443		3.61		C12H8F1N1S1	PHENOTHIAZINE,3-FLUORO
4246	N-HEPTANE	443		3.95		C12H8I1N1S1	PHENOTHIAZINE,3-IODO
4247	CYCLOHEXANE	141		1.87		C12H8N2	MALONONITRILE,CINNAMAL
4248	OCTANOL	283		1.83	1.83 =	C12H8N2.H2O	O-PHENANTHROLINE HYDRATE
4249	OCTANOL	218		2.84	2.84 =	C12H8N2	PHENAZINE
4250	CYCLOHEXANE	304		1.02		C12H8N2O2	MALONONITRILE,4-METHOXYCARBONYLBENZAL
4251	CYCLOHEXANE	304		1.35		C12H8N2O2	MALONONITRILE,2-METHOXYCARBONYLBENZAL
4252	OCTANOL	218		4.12	4.12 =	C12H8O1	DIBENZOFURAN
4253	CYCLOHEXANE	141		0.67		C12H8O3	1,4-NAPHTHOQUINONE,2-ACETYL
4254	CYCLOHEXANE	141		1.12		C12H8O4	1,4-NAPHTHOQUINONE,2-METHOXYCARBONYL
4255	CYCLOHEXANE	304		3.60		C12H9CL2N1O2	ETHYLCYANOACETATE,2,6-DICHLOROBENZAL
4256	OCTANOL	309		3.29	3.29 =	C12H9N1	CARBAZOLE
4257	N-HEPTANE	443		-1.09		C12H9N1O1S1	PHENOTHIAZINE,3-HYDROXY
4258	OCTANOL	141		1.29	1.29 =	C12H9N1O3	1,4-NAPHTHOQUINONE, 2-ACETAMIDO
4259	CYCLOHEXANE	141		0.13		C12H9N1O3	1,4-NAPHTHOQUINONE,2-ACETAMIDO
4260	OCTANOL	56		4.15	4.15 =	C12H9N1S1	PHENOTHIAZINE
4261	N-HEPTANE	443		3.88		C12H9N1S1	PHENOTHIAZINE
4262	OCTANOL	283	74	0.41	0.41 =	C12H9NA1O1	SODIUM P-PHENYLPHENOXIDE (PKA=9.51)
4263	OCTANOL	283		0.22	0.22 =	C12H9NA1O1	SODIUM P-PHENYLPHENOXIDE (PKA=9.51;PH=12.7)
4264	OCTANOL	56		4.09	4.09 =	C12H10	BIPHENYL
4265	OCTANOL	309		3.16	3.16 =	C12H10	BIPHENYL
4266	OCTANOL	428		4.04	4.04 =	C12H10	DIPHENYL
4267	CYCLOHEXANE	304		2.97		C12H10CL1N1O2	ETHYLCYANOACETATE,2-CHLOROBENZAL
4268	CYCLOHEXANE	304		3.54		C12H10CL1N1O2	ETHYLCYANOACETATE,3-CHLOROBENZAL
4269	CYCLOHEXANE	304		3.55		C12H10CL1N1O2	ETHYLCYANOACETATE,4-CHLOROBENZAL
4270	CYCLOHEXANE	141		1.24		C12H10CL1N1O2	1,4-NAPHTHOQUINONE,2-CHLORO,3-DIMETHYLAMINO
4271	CYCLOHEXANE	304		2.18		C12H10CL2O2	ACETYLACETONE,2,6-DICHLORO-BENZAL
4272	CYCLOHEXANE	304		2.75		C12H10F1N1O2	ETHYLCYANOACETATE,3-FLUROBENZAL
4273	OCTANOL	10		3.82	3.82 =	C12H10N2	AZOBENZENE
4274	CYCLOHEXANE	304		2.55		C12H10N2	MALONONITRILE,2-ETHYLBENZAL
4275	CYCLOHEXANE	304		2.23		C12H10N2O1	MALONONITRILE,4-ETHOXYBENZAL
4276	CYCLOHEXANE	304		2.55		C12H10N2O1	MALONONITRILE,3-ETHOXYBENZAL
4277	CYCLOHEXANE	304		2.70		C12H10N2O1	MALONONITRILE,2-ETHOXYBENZAL
4278	CYCLOHEXANE	141		1.05		C12H10N2O2	MALONONITRILE,3,4-DIMETHOXYBENZAL
4279	CYCLOHEXANE	141		2.02		C12H10N2O2	MALONONITRILE,2,4-DIMETHOXYBENZAL
4280	CYCLOHEXANE	304		1.08		C12H10N2O2	MALONONITRILE,3,4-DIMETHOXYBENZAL
4281	CYCLOHEXANE	141		-1.30		C12H10N2O3	1,4-NAPHTHOQUINONE,2-AMINO,3-ACETAMINO
4282	CYCLOHEXANE	304		1.74		C12H10N2O4	ETHYLCYANOACETATE,3-NITROBENZAL
4283	CHCL3	444	30	1.91	2.38 N	C12H10N4O6S1	N1-(3,5-DINITROPHENYL)SULFANILAMIDE
4284	OCTANOL	56		4.21	4.21 =	C12H10O1	DIPHENYL ETHER
4285	OCTANOL	276		4.36	4.36 =	C12H10O1	DIPHENYLETHER
4286	CYCLOHEXANE	445		1.94		C12H10O1	O-PHENYLPHENOL
4287	CYCLOHEXANE	133		0.98		C12H10O1	P-PHENYLPHENOL
4288	OCTANOL	141	26	2.49		C12H10O2	1,4-NAPHTHOQUINONE, 6,7-DIMETHYL
4289	CYCLOHEXANE	141		2.70		C12H10O2	1,4-NAPHTHOQUINONE,2,3-DIMETHYL
4290	OCTANOL	186		2.40	2.40 =	C12H10O2S1	SULFONE,DIPHENYL
4291	OCTANOL	10		2.53	2.53 =	C12H10O3	ACETIC ACIO,2-NAPHTHYLOXY
4292	OCTANOL	141	26	2.14		C12H10O3	1,4-NAPHTHOQUINONE,2-METHYL-3-METHOXY
4293	CYCLOHEXANE	141		2.31		C12H10O3	1,4-NAPHTHOQUINONE,2-METHYL,3-METHOXY
4294	CYCLOHEXANE	304		0.45		C12H10O4	COUMARIN-3-CARBOXYLIC ACIO,ETHYL ESTER
4295	CYCLOHEXANE	141		1.09		C12H10O4	1,4-NAPHTHOQUINONE,2,3-DIMETHOXY
4296	OCTANOL	276		3.47	3.47 =	C12H10S1	DIPHENYLSULFIDE
4297	OCTANOL	235		4.45	4.45 =	C12H10S1	DIPHENYLSULFIDE
4298	CHCL3	444	30	2.16	2.62 N	C12H11BR1N2O2S1	N1-(3-BROMOPHENYL)SULFANILAMIDE
4299	CYCLOHEXANE	304		1.82		C12H11BR1O2	ACETYLACETONE,4-BROMO-BENZAL
4300	CHCL3	444	30	1.97	2.44 N	C12H11CL1N2O2S1	N1-(3-CHLOROPHENYL)SULFANILAMIDE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4301	CYCLOHEXANE	304		1.67		C12H11CL1O2	ACETYLACETONE,4-CHLORO-BENZAL
4302	CYCLOHEXANE	304		1.69		C12H11CL1O2	ACETYLACETONE,3-CHLORO-BENZAL
4303	CYCLOHEXANE	304		1.99		C12H11CL1O2	ACETYLACETONE,2-CHLORO-BENZAL
4304	CYCLOHEXANE	304		0.95		C12H11F1O2	ACETYLACETONE,4-FLUORO-BENZAL
4305	CHCL3	444	30	2.47	2.71 N	C12H11I1N2O2S1	N1-(3-IODOPHENYL)SULFANILAMIDE
4306	PARAFFINS	316		2.10		C12H11N1	2-AMINOBIPHENYL
4307	PARAFFINS	316		1.67		C12H11N1	3-AMINOBIPHENYL
4308	PARAFFINS	316		1.74		C12H11N1	4-AMINOBIPHENYL
4309	OCTANOL	276		3.34	3.34 =	C12H11N1	DIPHENYLAMINE
4310	OCTANOL	309		3.22	3.22 =	C12H11N1	DIPHENYLAMINE
4311	OCTANOL	235		3.50	3.50 =	C12H11N1	DIPHENYLAMINE
4312	CYCLOHEXANE	141		2.63		C12H11N1O2	BENZALCYANOACETIC ACID,ETHYL ESTER
4313	CYCLOHEXANE	304		2.59		C12H11N1O2	BENZALCYANOACETIC ACID,ETHYL ESTER
4314	HEXANE	391		0.42		C12H11N1O2	N-METHYL CARBAMATE,1-NAPHTHYL
4315	OCTANOL	384		2.36	2.36 =	C12H11N1O2	N-METHYL-A-NAPHTHYLCARBAMATE
4316	OCTANOL	384		2.56	2.56 =	C12H11N1O2	N-METHYL-B-NAPHTHYLCARBAMATE
4317	DIETHYL ETHER	113		2.62	2.41 A	C12H11N1O2S1	BENZENESULFANILAMIDE
4318	CHCL3	113		2.87	3.29 N	C12H11N1O2S1	BENZENESULFANILAMIDE
4319	HEXANE	376		1.96		C12H11N1O2S1	N-ME-N-ACETYLCARBAMIC ACID,4-BENZOTHIENYL ESTER
4320	BENZENE	72		3.50	2.98 B	C12H11N3	P-AMINOAZOBENZENE
4321	CHCL3	444	30	2.44	2.88 N	C12H11N3O4S1	N1-(3-NITROPHENYL)SULFANILAMIDE
4322	CHCL3	444	30	1.52	2.02 N	C12H11N3O4S1	N1-(4-NITROPHENYL)SULFANILAMIDE
4323	OCTANOL	218		0.98	0.98 =	C12H11N7	PTERIDINE,2,4,7-TRIAMINO-6-PHENYL
4324	OCTANOL	65	46	-2.62	-2.62 =	C12H12BR1N1	BENZYLPYRIDINIUM BROMIDE
4325	CHCL3	444	30	1.45	1.96 N	C12H12N2O2S1	N1-PHENYLSULFANILAMIDE
4326	OCTANOL	80		1.42	1.42 =	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4327	CHCL3	399	1	0.65	1.20 N	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4328	OILS	82		0.23	1.43 A	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4329	OILS	345		0.13	1.37 A	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4330	OILS	398	44	0.00	1.19 A	C12H12N2O3	BARBITURIC ACID,5 ETHYL-5-PHENYL/PHENOBARBITAL/
4331	BENZENE	399	1	-0.01	1.40 A	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4332	I-PENT. ACETATE	399	1	1.54	1.42	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4333	CCL4	399	1	-0.63	1.31 A	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4334	OLEYL ALCOHOL	82		0.78	1.34	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4335	50%ETHER+50%DMF	125	12	-0.07	0.62	C12H12N2O3	BARBITURIC ACID,5-ETHYL-5-PHENYL/PHENOBARBITAL/
4336	CYCLOHEXANE	304		-1.63		C12H12N2O3	CYANOACETAMIDE,3,4-DIMETHOXYBENZAL
4337	CYCLOHEXANE	304		0.96		C12H12O2	ACETYLACETONE,BENZAL
4338	DIETHYL ETHER	414		0.87	0.87 A	C12H12O5	ADIPIC ACID,A-KETO-G-PHENYL
4339	N-HEPTANE	441		-2.13		C12H13CL1N2	8-CHLORO-9-METHYLTETRAHYDRO-B-CARBOLINE
4340	N-HEPTANE	441		-2.30		C12H13F1N2	6-FLUORO-9-METHYLTETRAHYDRO-B-CARBOLINE
4341	OCTANOL	206		4.27	4.27 =	C12H13F3N2	BENZIMIDAZOLE,5-BUTYL-2-(TRIFLUOROMETHYL)
4342	CYCLOHEXANE	446		-0.62		C12H13N1O1	N-CYCLOPROPYLCINNAMAMIDE
4343	CYCLOHEXANE	141		3.60		C12H13N1O2	1-CYCLOHEXENE,4-NITRO,5-PHENYL
4344	OCTANOL	235		2.14	2.14 =	C12H13N1O2S1	VITAVAX
4345	OCTANOL	283	65	1.49	1.49 =	C12H13N3O2	ISOCARBOXAZIDE
4346	OCTANOL	65	46	-2.52	-2.52 =	C12H14BR1N1	N-PROPYLQUINOLINIUM BROMIDE
4347	OILS	447		-0.03	1.22 A	C12H14BR1N1O3	A-BROMO-I-VALERYL-SALICYLAMIDE
4348	OILS	382	24	5.51	6.20 A	C12H14I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,AMYL ESTER
4349	OILS	382	24	2.76	3.70 A	C12H14I2O4	BENZOIC ACID,4-OH,3,5-DI-IODO,E-OH-AMYL ESTER
4350	N-HEPTANE	441		-1.99		C12H14N2	9-METHYLTETRAHYDRO-B-CARBOLINE
4351	50%ETHER+50%DMF	125		0.13	1.12	C12H14N2O4	5-FURFURYL-5-I-PROPYLBARBITURIC ACID/DORMOVIT/
4352	CYCLOHEXANE	304		-2.81		C12H14N2O4	MALONAMIDE,2,4-DIMETHOXYBENZAL
4353	MIXED SOLV#1	433		-2.70		C12H14N2O5	BARBITURIC ACID,1-CARBOXYMETHYL-5,5-DIALLYL
4354	OCTANOL	56		0.27	0.27 =	C12H14N4O2S1	SULFAMETHAZINE
4355	DIETHYL ETHER	113	15	-0.06	0.08 A	C12H14N4O2S1	SULFAMETHAZINE
4356	CHCL3	343	2	0.73	0.39 B	C12H14N4O2S1	SULFAMETHAZINE
4357	CHCL3	113	15	0.66	0.33 B	C12H14N4O2S1	SULFAMETHAZINE
4358	BENZENE	343	2	-0.43	0.03 B	C12H14N4O2S1	SULFAMETHAZINE
4359	I-PENT. ACETATE	343	2	0.56	0.40	C12H14N4O2S1	SULFAMETHAZINE
4360	CCL4	343	2	-1.35	0.72 A	C12H14N4O2S1	SULFAMETHAZINE
4361	OCTANOL	393	63	-0.30	-0.30 =	C12H14N4O2S1	SULFISOMIDINE
4362	DIETHYL ETHER	113	15	-1.06	0.71 B	C12H14N4O2S1	SULFISOMIDINE
4363	CHCL3	343	2	-0.55	0.09 N	C12H14N4O2S1	SULFISOMIDINE
4364	CHCL3	113	15	-0.69	-0.04 N	C12H14N4O2S1	SULFISOMIDINE
4365	CHCL3	393	63	-0.35	-0.33 N	C12H14N4O2S1	SULFISOMIDINE
4366	CHCL3	415	44	-0.52	0.12 N	C12H14N4O2S1	SULFISOMIDINE
4367	BENZENE	343	2	-1.21	0.18 A	C12H14N4O2S1	SULFISOMIDINE
4368	1-BUTANOL	130	13	1.74	1.94	C12H14N4O2S1	SULFISOMIDINE
4369	I-PENT. ACETATE	343	2	-0.40	-0.59	C12H14N4O2S1	SULFISOMIDINE
4370	CCL4	343	2	-1.89	0.25 A	C12H14N4O2S1	SULFISOMIDINE
4371	N-HEPTANE	415	44	-3.85		C12H14N4O2S1	SULFISOMIDINE
4372	OCTANOL	393	63	1.56	1.56 =	C12H14N4O4S1	SULFADIMETHOXINE
4373	CHCL3	343	2	1.49	2.01 N	C12H14N4O4S1	SULFADIMETHOXINE
4374	CHCL3	393	63	1.31	1.31 B	C12H14N4O4S1	SULFADIMETHOXINE
4375	BENZENE	343	2	0.70	2.08 A	C12H14N4O4S1	SULFADIMETHOXINE
4376	I-BUTANOL	130	13	2.48	2.93	C12H14N4O4S1	SULFADIMETHOXINE
4377	I-PENT. ACETATE	343	2	1.89	1.78	C12H14N4O4S1	SULFADIMETHOXINE
4378	CCL4	343	2	-0.63	1.31 A	C12H14N4O4S1	SULFADIMETHOXINE
4379	OCTANOL	134		1.73	1.73 =	C12H14N5O1	3-PHENYLAMINO-4-AMINO-6-I-PR-1,2,4-TRIAZINE-5-ONE
4380	OCTANOL	10		2.67	2.67 =	C12H14O3	2-(5,6,7,8-TETRAHYDRONAPHTHYLOXY-)ACETIC ACID
4381	CHCL3	194		-0.60	0.67 A	C12H14O4	ADIPIC ACID,B-PHENYL
4382	OCTANOL	438		0.26	0.26 =	C12H15CL1O6	GLUCOPYRANOSIDE,4-CHLOROPHENYL (BETA)
4383	OCTANOL	438		0.27	0.27 =	C12H15I1O6	GLUCOPYRANOSIDE,2-IODOPHENYL (BETA)
4384	OCTANOL	438		0.75	0.75 =	C12H15I1O6	GLUCOPYRANOSIDE,4-IODOPHENYL (BETA)
4385	HEXANE	376		0.92		C12H15N1O2	N-MECARBAMIC ACID,5,6,7,8-TETRAHYDRO-1-NAPHTHYL ESTER
4386	CYCLOHEXANE	141		3.52		C12H15N1O2	STYRENE,4-I-PROPYL,B-NITRO,B-METHYL
4387	HEXANE	391		2.20		C12H15N1O2S1	N-METHYL CARBAMATE,N-ACETYL,3-ME-4-METHYLTHIOPHENYL
4388	CYCLOHEXANE	141		2.17		C12H15N1O4	STYRENE,3,4-DIMETHOXY,B-NITRO,B-ETHYL
4389	CYCLOHEXANE	141		2.68		C12H15N1O4	STYRENE,2,4-DIMETHOXY,B-NITRO,B-ETHYL
4390	CYCLOHEXANE	141		2.68		C12H15N1O4	STYRENE,2,5-DIMETHOXY,B-NITRO,B-ETHYL
4391	CYCLOHEXANE	141		3.22		C12H15N1O4	STYRENE,2,3-DIMETHOXY,B-NITRO,B-ETHYL
4392	CYCLOHEXANE	141		2.24		C12H15N1O4	STYRENE,4-HYDROXY,3-ETHOXY,B-NITRO,B-ETHYL
4393	OCTANOL	438		-0.59	-0.59 =	C12H15N1O8	GALACTOPYRANOSIDE,4-NITROPHENYL (BETA)
4394	OCTANOL	438		-0.39	-0.39 =	C12H15N1O8	GLUCOPYRANOSIDE,4-NITROPHENYL (ALPHA)
4395	OCTANOL	438		-0.78	-0.78 =	C12H15N1O8	GLUCOPYRANOSIDE,2-NITROPHENYL (BETA)
4396	OCTANOL	438		-0.51	-0.51 =	C12H15N1O8	GLUCOPYRANOSIDE,3-NITROPHENYL (BETA)
4397	OCTANOL	438		-0.44	-0.44 =	C12H15N1O8	GLUCOPYRANOSIDE,4-NITROPHENYL (BETA)
4398	OCTANOL	438		-0.18	-0.18 =	C12H15N1O8	MANNOPYRANOSIDE,4-NITROPHENYL(ALPHA)
4399	MIXED SOLV#1	433		-0.82		C12H15N3O4	BARBITURIC ACID,1-CARBAMYLMETHYL-5,5-DIALLYL
4400	OILS	447		-0.02	1.23 A	C12H16BR1N1O2	A-BROMO-I-VALERYL-O-ANISIDINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT.	EMPIRICAL FORMULA	NAME
4401	N-HEPTANE	416	14	1.12		C12H16CL1N1O3	P-AMINOSALICYLIC ACID,5-CHLOROAMYL ESTER
4402	CHCL3	396	31	3.22	2.53 B	C12H16F3N1	FENFLURAMINE
4403	N-HEPTANE	138		2.74		C12H16F3N1	FENFLURAMINE
4404	N-HEPTANE	396	31	2.83		C12H16F3N1	FENFLURAMINE
4405	CCL4	306		0.20	2.02 A	C12H16I1N1O4S1	N-(P-IODOBENZENESULFONYL)-L-LEUCINE
4406	CCL4	306		0.09	1.92 A	C12H16I1N1O4S1	N-(P-IODOBENZENESULFONYL)LEUCINE
4407	OCTANOL	341	60	1.49	1.49 =	C12H16N2	3-PYRIDYLMETHYL-N-PIPERIDINE
4408	CHCL3	448	65	-1.22		C12H16N2O2	N,N-DIMETHYLTRYPTAMINE, 5-HYDROXY
4409	CHCL3	448	65	0.74		C12H16N2O2	N,N-DIMETHYLTRYPTAMINE, 4-HYDROXY
4410	OCTANOL	218		1.20	1.20 =	C12H16N2O3	CYCLOBARBITAL
4411	50%ETHER+50%DMF	125		0.15	1.17	C12H16N2O3	CYCLOBARBITAL
4412	OCTANOL	218		1.49	1.49 =	C12H16N2O3	HEXOBARBITAL
4413	CHCL3	399	1	2.11	1.58 B	C12H16N2O3	HEXOBARBITAL
4414	I-PENT. ACETATE	399	1	1.86	1.75	C12H16N2O3	HEXOBARBITAL
4415	CCL4	399	1	0.88		C12H16N2O3	HEXOBARBITAL
4416	50%ETHER+50%DMF	125	12	0.46	1.95	C12H16N2O3	HEXOBARBITAL
4417	SEC-BUTANOL	84	19	-2.05	-3.38	C12H16N6O3	HISTIDYLHISTIDINE
4418	OILS	361		1.25	2.40 A	C12H16O2	6-PHENYLCAPROIC ACID
4419	OCTANOL	10		3.18	3.18 =	C12H16O3	PHENOXYACETIC ACID,3-BUTYL
4420	OCTANOL	10		3.12	3.12 =	C12H16O3	PHENOXYACETIC ACID,4-S-BUTYL
4421	OCTANOL	10		2.96	2.96 =	C12H16O3	PHENOXYACETIC ACID,3-T-BUTYL
4422	OCTANOL	438		-0.71	-0.71 =	C12H16O6	GLUCOPYRANOSIDE, PHENYL (BETA)
4423	DIETHYL ETHER	3		-3.13	-2.62 A	C12H16O7	B-D-GLUCOPYRANOSIDE,P-HYDROXYPHENYL/ARBUTIN/
4424	OCTANOL	438		-1.35	-1.35 =	C12H16O7	B,D-GLUCOPYRANOSIDE,P-HYDROXYPHENYL/ARBUTIN/
4425	I-BUTANOL	4		-0.55	-1.28	C12H16O7	B,D-GLUCOPYRANOSIDE,P-HYDROXYPHENYL/ARBUTIN/
4426	50%ETHER+50%DMF	125		0.46	1.95	C12H17BR1N2O3	5-(2-BROMALLYL)-5-(1-METHYLBUTYL)-BARBITURIC ACID
4427	CHCL3	396	31	3.38	2.66 B	C12H17N1O1	PHENDIMETRAZINE
4428	N-HEPTANE	396	31	0.95		C12H17N1O1	PHENDIMETRAZINE
4429	I-PENT. ACETATE	418	3	4.41	4.40	C12H17N1O2	P-AMINOBENZOIC ACID,N-AMYL ESTER
4430	OLEYL ALCOHOL	390	44	3.24	3.78	C12H17N1O2	P-AMINOBENZOIC ACID,PENTYL ESTER
4431	HEXANE	376		1.79		C12H17N1O2	N,N-DIMETHYLCARBAMIC ACID,M-I-PROPYLPHENYL ESTER
4432	HEXANE	391		1.56		C12H17N1O2	N-METHYL CARBAMATE,3-I-PROPYL,5-METHYLPHENYL
4433	HEXANE	391		1.54		C12H17N1O2	N-METHYL CARBAMATE,3-S-BUTYLPHENYL
4434	HEXANE	391		1.48		C12H17N1O2	N-METHYL CARBAMATE,3-T-BUTYL PHENYL
4435	OCTANOL	384		2.78	2.78 =	C12H17N1O2	N-METHYL-2-S-BUTYLPHENYLCARBAMATE
4436	OCTANOL	384		2.65	2.65 =	C12H17N1O2	N-METHYL-2-T-BUTYLPHENYLCARBAMATE
4437	OCTANOL	384		3.11	3.11 =	C12H17N1O2	N-METHYL-3-METHYL-4-I-PROPYLPHENYLCARBAMATE
4438	OCTANOL	384		3.10	3.10 =	C12H17N1O2	N-METHYL-3-METHYL-5-I-PROPYLPHENYLCARBAMATE
4439	OCTANOL	384		2.84	2.84 =	C12H17N1O2	N-METHYL-3-METHYL-6-I-PROPYLPHENYLCARBAMATE
4440	OCTANOL	384		2.93	2.93 =	C12H17N1O2	N-METHYL-3-T-BUTYLPHENYLCARBAMATE
4441	OCTANOL	384		3.20	3.20 =	C12H17N1O2	N-METHYL-4-S-BUTYLPHENYLCARBAMATE
4442	OCTANOL	384		3.06	3.06 =	C12H17N1O2	N-METHYL-4-T-BUTYLPHENYLCARBAMATE
4443	OLEYL ALCOHOL	142		1.47	2.02	C12H17N1O2	PHENOXYACETAMIDE,N,N-DIETHYL
4444	N-HEPTANE	370	14	1.32		C12H17N1O3	P-AMINOSALICYLIC ACID,N-AMYL ESTER
4445	OCTANOL	384		2.96	2.96 =	C12H17N1O3	N-METHYL-3-BUTOXYPHENYLCARBAMATE
4446	N-HEPTANE	370	14	0.28		C12H17N1O4	P-AMINOSALICYLIC ACID,5-HYDROXYAMYL ESTER
4447	OCTANOL	438		-2.67	-2.67 =	C12H17N1O6	GLUCOPYRANOSIDE,4-AMINOPHENYL (BETA)
4448	OCTANOL	438		-1.23	-1.23 =	C12H17N1O6	GLUCOPYRANOSIDE,2-AMINOPHENYL (BETA)
4449	OCTANOL	341	60	1.66	1.66 =	C12H18N2	3-PYRIDYLETHYL-2-(N-PIPERIDINE)
4450	N-HEPTANE	400	14	-1.40		C12H18N2O1.HCL	OXO-TREMORINE
4451	N-HEPTANE	419		0.35		C12H18N2O1	UREA,N-BUTYL,O-TOLYL-
4452	N-HEPTANE	419		0.12		C12H18N2O1	UREA,N-BUTYL,P-TOLYL-
4453	OCTANOL	449		1.95	1.95 =	C12H18N2O2	BENZOIC ACID,P-ME-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4454	OILS	449		0.90	2.01 A	C12H18N2O2	BENZOIC ACID,P-ME-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4455	XYLENE	449		1.38		C12H18N2O2	BENZOIC ACID,P-ME-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4456	DI-BUTYL ETHER	449		1.01		C12H18N2O2	BENZOIC ACID,P-ME-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4457	CHCL3	399	1	2.84	3.30 N	C12H18N2O2S1	BARBITURIC ACID,5-ALLYL-5-I-AMYL,2-THIO
4458	I-PENT. ACETATE	399	1	3.23	3.17	C12H18N2O2S1	BARBITURIC ACID,5-ALLYL-5-I-AMYL,2-THIO
4459	CCL4	399	1	1.84	3.43 A	C12H18N2O2S1	BARBITURIC ACID,5-ALLYL-5-I-AMYL,2-THIO
4460	OCTANOL	218		3.23	3.23 =	C12H18N2O2S1	BARBITURIC ACID,5-ALLYL-5-(1-MEBUTYL)2-THIO
4461	OLEYL ALCOHOL	142		2.50	3.04	C12H18N2O2S1	BARBITURIC ACID,5-ALLYL-5(1-MEBUTYL),2-THIO
4462	CHCL3	399		2.27	2.75 N	C12H18N2O2S1	BARBITURIC ACID,5-(CYCLOHEX-1-YL),5-ET,2-THIO (1)
4463	I-PENT. ACETATE	399	1	2.75	2.67	C12H18N2O2S1	BARBITURIC ACID,5-(CYCLOHEX-1YL)-5-ET-2-THIO
4464	CCL4	399		1.17	2.80 A	C12H18N2O2S1	BARBITURIC ACID,5-(CYCLOHEX-1-YL),5-ET,2-THIO (1)
4465	50%ETHER+50%DMF	125		0.62	2.34	C12H18N2O3	BARBITURIC ACID,5-ALLYL-5-(1-MEBUTYL)/SECOBARBITAL/
4466	PRIM. PENTANOLS	181	10	-0.15		C12H19CL1N4O7P2S1	THIAMINE PYROPHOSPHATE /COCARBOXYLASE/
4467	CHCL3	396	31	3.68	2.92 B	C12H19N1	METHYLETHYLAMPHETAMINE
4468	N-HEPTANE	396	31	2.22		C12H19N1	METHYLETHYLAMPHETAMINE
4469	DIETHYL ETHER	374		2.11	2.71 B	C12H19N1	N-PROPYL-G-PHENYLPROPYLAMINE
4470	CHCL3	396	31	3.91	3.12 B	C12H19N1	PROPYLAMPHETAMINE
4471	N-HEPTANE	138		2.56		C12H19N1	PROPYLAMPHETAMINE
4472	N-HEPTANE	396	31	2.49		C12H19N1	PROPYLAMPHETAMINE
4473	CHCL3	396	31	3.65	2.90 B	C12H19N1	I-PROPYLAMPHETAMINE
4474	N-HEPTANE	396	31	2.07		C12H19N1	I-PROPYLAMPHETAMINE
4475	OCTANOL	227		0.06	0.06 =	C12H19N3O1.H1CL1	PROCARBAZINE HYDROCHLORIDE (77213)(PKA= 6.66)
4476	OCTANOL	437		2.73	2.73 =	C12H19O4P1S1	O,O-DIETHYL-O-(3-ME-4-METHIOPHENYL)PHOSPHATE
4477	OCTANOL	437		2.82	2.82 =	C12H19O6P1S1	O,O-DIETHYL-O-(2-ME-4-MESULFONYLPHENYL)PHOSPHATE
4478	OCTANOL	255		-2.02		C12H20I1N1	G-PHENYLPROPYL-TRIMETHYL-AMMONIUM IODIDE
4479	OCTANOL	341	60	2.27	2.27 =	C12H20N2	N,N-DI-I-PROPYL-3-PRYIDYLMETHYLAMINE
4480	OCTANOL	341	60	1.46	1.46 =	C12H20N2	N,N-DIPROPYL-3-PYRIDYLMETHYLAMINE
4481	CHCL3	322		2.00	2.38 N	C12H20N2O2S2	BARBITURIC ACID,5-(1-MEBU)-5-(2-METHIO)-2-THIO
4482	OILS	442		2.04	3.04 A	C12H20N2O2S2	BARBITURIC ACID,5-(1-MEBU)-5-(2-METHIO)-2-THIO
4483	CHCL3	399	1	2.74	2.15 B	C12H20N2O3	BARBITURIC ACID,5-ET-5-I-AMYL-N-METHYL
4484	I-PENT. ACETATE	399	1	2.61	2.52	C12H20N2O3	BARBITURIC ACID,5-ET-5-I-AMYL-N-METHYL
4485	CCL4	399	1	1.95		C12H20N2O3	BARBITURIC ACID,5-ET-5-I-AMYL-N-METHYL
4486	DIETHYL ETHER	3		0.65	0.67 A	C12H20O7	CITRIC ACID,TRIETHYL ESTER
4487	OILS	2		-0.30	0.97 A	C12H20O7	CITRIC ACID,TRIETHYL ESTER
4488	PRIM. PENTANOLS	263		0.41	0.13	C12H21N6O6CO1	TRI-(2,3-BUTANEDIONEOXIME) COBALT
4489	OCTANOL	438		-0.63	-0.63 =	C12H22O6	GLUCOPYRANOSIDE,CYCLOHEXYL (BETA)
4490	I-BUTANOL	4		-2.40	-3.88	C12H22O11	MALTOSE
4491	I-BUTANOL	4		-2.25	-3.67	C12H22O11	SUCROSE
4492	OCTANOL	260		1.72	1.72 =	C12H23N1O1	2-AZATRIDECANONE
4493	DIETHYL ETHER	378	44	-0.36	0.62 B	C12H24N2O2	PIPERIDINYL FORMIC ACID,DIETAMINOETHYL ESTER
4494	OCTANOL	218	26	4.20		C12H24O2	DODECANOIC ACID/LAURIC ACID/
4495	N-HEPTANE	139	31	3.03		C12H24O2	DODECANOIC ACID/LAURIC ACID/
4496	SEC-BUTANOL	84	19	-0.75	-1.56	C12H25N5O3	ARGINYLLEUCINE
4497	OCTANOL	268	32	1.60	1.60 =	C12H25NA1O4S1	DODECYL SULFATE,SODIUM SALT
4498	N-BUTANOL	450		0.25	-0.13	C12H26N4O6	NEAMINE/NEOMYCIN A/(AS 2-ETHYL BUTYRATE)
4499	OCTANOL	218		5.13	5.13 =	C12H26O1	1-DODECANOL
4500	DIETHYL ETHER	2		-1.21	-0.95 A	C12H26O5	TETRAETHYLENE GLYCOL DIETHYL ETHER

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4501	CHCL3	451	12	2.05	1.52	C12H27N1	TRIBUTYLAMINE
4502	TOLUENE	452		0.58	1.04 B	C12H27O1P1	TRIBUTYL PHOSPHINE OXIDE
4503	OCTANOL	268	46	1.85	1.85 =	C12H28CL1N1	DODECYLAMINE HYDROCHLORIDE
4504	50%ETHER+50%DMF	125		0.34	1.65	C13N14N2O3	BARBITURIC ACID, 5-ETHYL-5-PHENYL-N-METHYL
4505	CYCLOHEXANE	304		2.28		C13H7F3N2	MALONONITRILE,2-TRIFLUOROMETHYLCINNAMAL
4506	CYCLOHEXANE	304		2.98		C13H8O1	9-FLUORENONE
4507	OCTANOL	427		3.40	3.40 =	C13H9N1	ACRIDINE
4508	OILS	453	50	2.30	3.29 A	C13H9N1	ACRIDINE
4509	OCTANOL	283	71	-0.27	-0.27 =	C13H9NA1O2	P-BIPHENYLCARBOXYLIC ACID, SODIUM SALT
4510	OCTANOL	283	72	0.77	0.77 =	C13H9NA1O2	BIPHENYLCARBOXYLIC ACID, SODIUM SALT
4511	OCTANOL	283	73	-0.38	-0.38 =	C13H9NA1O2	BIPHENYLCARBOXYLIC ACID, SODIUM SALT
4512	OCTANOL	216	46	-0.50	-0.50 =	C13H10CL1N1	ACRIDINE HYDROCHLORIDE
4513	N-HEPTANE	443		1.42		C13H10CL1N1O1S1	PHENOTHIAZINE,2-CHLORO,7-METHOXY
4514	OCTANOL	218		4.70	4.70 =	C13H10CL2N2O1	UREA,1-(3,4-DICHLOROPHENYL)-3-PHENYL
4515	OCTANOL	346		2.47	2.47 =	C13H10N2	1-AMINOACRIDINE
4516	OILS	453		1.79	2.92 A	C13H10N2	1-AMINOACRIDINE
4517	OCTANOL	346		2.62	2.62 =	C13H10N2	2-AMINOACRIDINE
4518	OILS	453		1.97	3.08 A	C13H10N2	2-AMINOACRIDINE
4519	OCTANOL	346		2.19	2.19 =	C13H10N2	3-AMINOACRIDINE
4520	OILS	453	12	1.87	3.00 A	C13H10N2	3-AMINOACRIDINE
4521	OCTANOL	346		3.26	3.26 =	C13H10N2	4-AMINOACRIDINE
4522	OILS	453	12	3.08	4.00 A	C13H10N2	4-AMINOACRIDINE
4523	OCTANOL	216		2.74	2.74 =	C13H10N2	9-AMINOACRIDINE
4524	PARAFFINS	439		0.85		C13H10N2	9-AMINOPHENANTHRIDINE
4525	CYCLOHEXANE	304		1.29		C13H10N2O2	ETHYLCYANOACETATE,4-CYANOBENZAL
4526	OCTANOL	218		0.33	0.33 =	C13H10N2O4	PHTHALIMIDE,N-(2,6-DIOXO-3-PIPERIDYL)
4527	OCTANOL	235		3.18	3.18 =	C13H10O1	BENZOPHENONE
4528	OCTANOL	235		3.18	3.18 =	C13H10O1	BENZOPHENONE
4529	CHCL3	388		3.90	4.76 A	C13H10O2SE1	1-(2-SELENOPHEN-YL)-3-PHENYL-1,3-PROPANEDIONE
4530	BENZENE	388		3.66	4.94 A	C13H10O2SE1	1-(2-SELENOPHEN-YL)-3-PHENYL-1,3-PROPANEDIONE
4531	TOLUENE	148		2.52	2.50 B	C13H11CU1N4O1	CUPROUS-CARBAZONE COMPLEX
4532	TOLUENE	148		0.81	1.21 B	C13H11HG1N4O1	MERCURIC-CARBAZONE COMPLEX
4533	TOLUENE	148		2.00	2.10 B	C13H11HG2N4O1	MERCUROUS-CARBAZONE COMPLEX
4534	PARAFFINS	316		1.76		C13H11N1	2-AMINOFLUORENE
4535	OCTANOL	56		2.62	2.62 =	C13H11N1O1	BENZANILIDE
4536	OCTANOL	9	26	3.09	3.09 =	C13H11N1O1	SALICYLALDEHYDE-ANIL
4537	N-HEPTANE	443		2.43		C13H11N1O1S1	PHENOTHIAZINE,3-METHOXY
4538	OCTANOL	238		3.27	3.27 =	C13H11N1O2	SALICYLANILIDE
4539	N-HEPTANE	443		3.23		C13H11N1S1	PHENOTHIAZINE,3-METHYL
4540	N-HEPTANE	443		4.58		C13H11N1S1	PHENOTHIAZINE,10-METHYL
4541	OCTANOL	346		1.10	1.10 =	C13H11N3	2,8-DIAMINOACRIDINE
4542	OCTANOL	235		4.14	4.14 =	C13H12	DIPHENYLMETHANE
4543	CYCLOHEXANE	304		1.91		C13H12CL2O3	ETHYLACETOACETATE,2,6-DICHLOROBENZAL
4544	CYCLOHEXANE	304		2.98		C13H12CL2O3	ETHYLACETOACETATE,2,4-DICHLOROBENZAL
4545	CYCLOHEXANE	304		4.00		C13H12CL2O3	ETHYLACETOACETATE,3,4-DICHLOROBENZAL
4546	CYCLOHEXANE	304		3.33		C13H12N2O1	MALONONITRILE,2-I-PROPOXYBENZAL
4547	TOLUENE	454		1.59		C13H12N4O1	DIPHENYLCARBAZONE
4548	CCL4	454		0.88		C13H12N4O1	DIPHENYLCARBAZONE
4549	CHCL3	455	12	5.90		C13H12N4S1	DIPHENYLTHIOCARBAZONE/DITHIZONE/
4550	CCL4	203		1.61		C13H12N4S1	DIPHENYLTHIOCARBAZONE/DITHIZONE/
4551	OCTANOL	276		2.03	2.03 =	C13H12O1	DIPHENYLCARBINOL
4552	OCTANOL	428		2.67	2.67 =	C13H12O1	DIPHENYLCARBINOL
4553	HEXANE	456		0.56		C13H12O3	GRISAN-3,4'-DIONE
4554	CYCLOHEXANE	304		2.23		C13H13F1O3	ETHYLACETOACETATE,3-FLUOROBENZAL
4555	CYCLOHEXANE	304		3.26		C13H13N1O2	ETHYLCYANOACETATE,2-METHYLBENZAL
4556	CYCLOHEXANE	304		3.62		C13H13N1O2	ETHYLCYANOACETATE,4-METHYLBENZAL
4557	HEXANE	376		2.45		C13H13N1O2S1	N-ME-N-PROPIONYLCARBAMIC ACID,4-BENZOTHIENYL ESTER
4558	DIETHYL ETHER	113		0.67	0.70 A	C13H13N1O2S1	N-P-TOLUENEBENZENESULFONAMIDE
4559	CHCL3	113		0.43	1.77 A	C13H13N1O2S1	N-P-TOLUENEBENZENESULFO AMIDE
4560	CYCLOHEXANE	304		2.47		C13H13N1O3	ETHYLCYANOACETATE,4-METHOXYBENZAL
4561	CYCLOHEXANE	304		2.68		C13H13N1O3	ETHYLCYANOACETATE,2-METHOXYBENZAL
4562	CYCLOHEXANE	304		2.80		C13H13N1O3	ETHYLCYANOACETATE,3-METHOXYBENZAL
4563	OCTANOL	65	46	-2.35	-2.35 =	C13H14BR1N1	B-PHENYLETHYLPYRIDINIUM BROMIDE
4564	DIETHYL ETHER	457	62	0.39	0.46 A	C13H14N2O2	1,4-NAPHTHOQUINONE,2-I-PROPYLHYDRAZINO
4565	CHCL3	444	30	2.00	2.47 N	C13H14N2O2S1	N1-(4-METHYLPHENYL)SULFANILAMIDE
4566	CHCL3	399	1	1.98	1.37 B	C13H14N2O3	BARBITURIC ACID,1-ME,5-ET,5-PHENYL
4567	I-PENT. ACETATE	399	1	1.75	1.64	C13H14N2O3	BARBITURIC ACID,1-ME,5-ET,5-PHENYL
4568	CCL4	399	1	0.80		C13H14N2O3	BARBITURIC ACID,1-ME,5-ET,5-PHENYL
4569	CHCL3	444	30	1.64	2.13 N	C13H14N2O3S1	N1-(3-METHOXYPHENYL)SULFANILAMIDE
4570	CYCLOHEXANE	304		1.52		C13H14O2	ACETYLACETONE,2-METHYL BENZAL
4571	CYCLOHEXANE	304		1.57		C13H14O2	ACETYLACETONE,4-METHYL BENZAL
4572	CYCLOHEXANE	304		0.91		C13H14O3	ACETYLACETONE,4-METHOXY-BENZAL
4573	CYCLOHEXANE	304		1.04		C13H14O3	ACETYLACETONE,2-METHOXY-BENZAL
4574	CYCLOHEXANE	304		1.06		C13H14O3	ACETYLACETONE,3-METHOXY-BENZAL
4575	CYCLOHEXANE	304		2.03		C13H14O3	ETHYLACETOACETATE,BENZAL
4576	OCTANOL	438		0.49	0.49 =	C13H15F3O6	GLUCOPYRANOSIDE,3-TRIFLUOROMETHYLPHENYL(BETA)
4577	OCTANOL	218		1.90	1.90 =	C13H15N1O2	GLUTARIMIDE,2-ETHYL-2-PHENYL
4578	HEXANE	376		1.15		C13H15N1O2	N-MECARBAMIC ACID,O-CYCLOPENTENYLPHENYL ESTER
4579	CHCL3	67		-0.84		C13H15N1O5	D,L-TYROSINE,O,N-DIACETYL
4580	CHCL3	338	44	0.18	-0.08 B	C13H15N3O2	N-ACETYL-4-AMINOANTIPYRINE
4581	BENZENE	338	44	-2.70		C13H15N3O2	N-ACETYL-4-AMINOANTIPYRINE
4582	N-HEPTANE	338	44	-2.40		C13H15N3O2	N-ACETYL-4-AMINOANTIPYRINE
4583	OILS	382	24	6.02	6.66 A	C13H16I2O3	BENZOIC ACID,4-OH,3,5-DI-IODO,HEXYL ESTER
4584	OILS	382	24	3.30	4.19 A	C13H16I2O4	BENZOIC ACID,3,5-DI-IODO-4-OH,6-OH-HEXYL ESTER
4585	MIXED SOLV#1	433		1.18		C13H16N2O3	BARBITURIC ACID,I-ALLYL-5,5-DIALLYL
4586	OCTANOL	10		3.41	3.41 =	C13H16O3	PHENOXYACETIC ACID,4-CYCLOPENTYL
4587	HEXANE	376		1.38		C13H17N1O2	N-METHYLCARBAMIC ACID,O-CYCLOPENTYLPHENYL ESTER
4588	CYCLOHEXANE	141		2.89		C13H17N1O2	STYRENE,4-I-PROPYL,B-NITRO,B-ETHYL
4589	OCTANOL	458		1.59	1.59 =	C13H17N1O3	5-(A,A-DIETHYLACETAMIDO)-1,3-BENZODIOXOLE
4590	HEXANE	376		2.53		C13H17N1O3	N-METHYL-N-ACETYLCARBAMIC ACID,M-I-PROPYLPHENYL ESTER
4591	HEXANE	376		1.84		C13H17N1O4	N-ME-N-ACETYLCARBAMIC ACID,O-I-PROPOXYPHENYL ESTER
4592	CYCLOHEXANE	141		2.45		C13H17N1O4	STYRENE,3,4-DIETHOXY,B-METHYL-B-NITRO
4593	OCTANOL	218		0.80	0.80 =	C13H17N3O1	AMINOPYRINE
4594	DIETHYL ETHER	3		-0.20	0.67 B	C13H17N3O1	AMINOPYRINE
4595	CHCL3	338	44	1.86	1.36 B	C13H17N3O1	AMINOPYRINE
4596	CHCL3	405		1.47	1.03 B	C13H17N3O1	AMINOPYRINE
4597	OILS	2		-0.59	0.71 A	C13H17N3O1	AMINOPYRINE
4598	BENZENE	338	44	-0.40		C13H17N3O1	AMINOPYRINE
4599	BENZENE	405		0.83	1.12 B	C13H17N3O1	AMINOPYRINE
4600	N-HEPTANE	254		-0.68		C13H17N3O1	AMINOPYRINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4601	N-HEPTANE	338	44	-0.82		C13H17N3O1	AMINOPYRINE
4602	N-HEPTANE	340		-0.68		C13H17N3O1	AMINOPYRINE
4603	OLEYL ALCOHOL	82		0.11	0.67	C13H17N3O1	AMINOPYRINE
4604	N-HEPTANE	416	14	1.17		C13H18CL1N1O3	P-AMINOSALICYLIC ACID,6-CHLOROHEXYL ESTER
4605	N-HEPTANE	138		3.45		C13H18F3N1	N-PROPYLNORFENFLURAMINE
4606	CHCL3	448	65	0.36		C13H18N2O1	N,N-DIMETHYLTRYPTAMINE,4-METHOXY
4607	CHCL3	448	65	0.52		C13H18N2O1	N,N-DIMETHYLTRYPTAMINE,5-METHOXY
4608	CHCL3	448	65	0.57		C13H18N2O1	N,N-DIMETHYLTRYPTAMINE,6-METHOXY
4609	CHCL3	448	65	0.98		C13H18N2O1	N,N-DIMETHYLTRYPTAMINE,7-METHOXY
4610	50%ETHER+50%DMF	125		0.26	1.45	C13H18N2O3	BARBITURIC ACID, 5-(1-CYCLOHEPTEN-1-YL)-5-ETHYL
4611	CHCL3	399	1	2.48	1.92 B	C13H18N2O3	CYCLOBARBITAL,N-METHYL
4612	I-PENT. ACETATE	399	1	2.27	2.18	C13H18N2O3	CYCLOBARBITAL,N-METHYL
4613	CCL4	399	1	1.49		C13H18N2O3	CYCLOBARBITAL,N-METHYL
4614	OCTANOL	56		4.35	4.35 =	C13H18O3	P-HYDROXYBENZOIC ACID,HEXYL ESTER
4615	OCTANOL	438		-0.70	-0.70 =	C13H18O6	GLUCOPYRANOSIDE,BENZYL (BETA)
4616	OCTANOL	438		-0.20	-0.20 =	C13H18O6	GLUCOPYRANOSIDE,3-METHYLPHENYL (BETA)
4617	OCTANOL	438		-0.16	-0.16 =	C13H18O6	GLUCOPYRANOSIDE,2-METHYLPHENYL (BETA)
4618	OCTANOL	438		-0.16	-0.16 =	C13H18O6	GLUCOPYRANOSIDE,4-METHYLPHENYL (BETA)
4619	OCTANOL	438		-1.22	-1.22 =	C13H18O7	GLUCOPYRANOSIDE,2-HYDROXYMETHYLPHENYL(BETA)
4620	OCTANOL	438		-1.04	-1.04 =	C13H18O7	GLUCOPYRANOSIDE,2-METHOXYPHENYL (BETA)
4621	OCTANOL	438		-0.73	-0.73 =	C13H18O7	GLUCOPYRANOSIDE,4-METHOXYPHENYL (BETA)
4622	OCTANOL	438		-0.52	-0.52 =	C13H18O7	GLUCOPYRANOSIDE,3-METHOXYPHENYL (BETA)
4623	1-BUTANOL	4		-0.40	-1.07	C13H18O7	GLUCOPYRANOSIDE,SALICYL ALCOHOL
4624	OLEYL ALCOHOL	390	44	3.71	4.25	C13H19N1O2	P-AMINOBENZOIC ACID,HEXYL ESTER
4625	OCTANOL	384		3.38	3.38 =	C13H19N1O2	N-METHYL-3-METHYL-4-T-BUTYLPHENYLCARBAMATE
4626	OCTANOL	384		3.35	3.35 =	C13H19N1O2	N-METHYL-3-METHYL-5-T-BUTYLPHENYLCARBAMATE
4627	OCTANOL	384		3.14	3.14 =	C13H19N1O2	N-METHYL-3-METHYL-6-T-BUTYLPHENYLCARBAMATE
4628	N-HEPTANE	370	14	1.40		C13H19N1O3	P-AMINOSALICYLIC ACID,N-HEXYL ESTER
4629	OLEYL ALCOHOL	142		0.89	1.45	C13H19N1O3	2-METHOXY-PHENOXYACETAMIDE,N,N-DIETHYL
4630	N-HEPTANE	370	14	0.50		C13H19N1O4	P-AMINOSALICYLIC ACID,6-HYDROXYHEXYL ESTER
4631	OCTANOL	276		4.14	4.14 =	C13H20CL1N2	N-DIETHYLAMINOETHYLANILINE,3-CL-4-METHYL /PKA= 9.6/
4632	OLEYL ALCOHOL	459	31	2.57	3.14	C13H20N2O1S1	THIOCAINE
4633	OLEYL ALCOHOL	460		1.90	2.45	C13H20N2O2	P-AMINOBENZOIC ACID,DIETHYLAMINO-ETHYL ESTER
4634	OCTANOL	449		2.62	2.62 =	C13H20N2O2	BENZOIC ACID,P-ET.AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4635	OILS	449		1.46	2.52 A	C13H20N2O2	BENZOIC ACID,P-ET-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4636	XYLENE	449		2.20		C13H20N2O2	BENZOIC ACID,P-ET-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4637	DI-BUTYL ETHER	449		1.65		C13H20N2O2	BENZOIC ACID,P-ET-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4638	DIETHYL ETHER	378	44	0.50	1.38 B	C13H20N2O2	N-PHENYLCARBAMIC ACID,DIETAMINOETHYL ESTER
4639	OCTANOL	218		1.87	1.87 =	C13H20N2O2	PROCAINE
4640	OCTANOL	218		1.92	1.92 =	C13H20N2O2	PROCAINE
4641	DIETHYL ETHER	461		1.81	1.71 A	C13H20N2O2	PROCAINE /NOVOCAINE/
4642	CHCL3	405	31	2.66	2.08 B	C13H20N2O2	PROCAINE /NOVOCAINE/
4643	OILS	462		1.82	1.93 B	C13H20N2O2	PROCAINE
4644	1-BUTANOL	4		1.80	2.03	C13H20N2O2	PROCAINE
4645	OLEYL ALCOHOL	459	31	1.79	2.35	C13H20N2O2	PROCAINE /NOVOCAINE/
4646	OCTANOL	235		-2.24	-2.24 =	C13H20N2O2	PROCAINE (PH=3.8;PKA(1)=8.96;PKA(2)=2.01)
4647	OCTANOL	235		0.16	0.16 =	C13H20N2O2	PROCAINE (PH=7.30;PKA=8.96)
4648	DIETHYL ETHER	3		0.97	1.70 B	C13H20O8	PENTAERITHRITOL TETRA-ACETATE
4649	I-BUTANOL	4		0.97	0.87	C13H20O8	PENTAERITHRITOL TETRAACETATE
4650	OCTANOL	373		-0.67	-0.67 =	C13H21CL1N2O1	N1-HEPTYLNICOTINAMIDE CHLORIDE
4651	DIETHYL ETHER	374		2.43	3.02 B	C13H21N1	N-BUTYL-G-PHENYLPROPYL AMINE
4652	N-HEPTANE	138		3.10		C13H21N1	N-BUTYLAMPHETAMINE
4653	CHCL3	396	31	4.05	3.24 B	C13H21N1	METHYL-1-PROPYLAMPHETAMINE
4654	N-HEPTANE	396	31	2.30		C13H21N1	METHYL-1-PROPYLAMPHETAMINE
4655	OLEYL ALCOHOL	459	31	1.27	1.84	C13H21N3O1	B-DIETAMINOPROPIONAMIDE,N-(P-AMINOPHENYL)
4656	OLEYL ALCOHOL	459	31	1.22	1.77	C13H21N3O1	PROCAINEAMIDE
4657	OCTANOL	65	46	-1.85	-1.85 =	C13H22BR1N1	BENZYLDIMETHYLBUTYLAMMONIUM BROMIDE
4658	OCTANOL	65	53	-0.95	-0.95 =	C13H22BR1N1	OCTYLPYRIDINIUM BROMIDE
4659	OLEYL ALCOHOL	459	31	1.65	2.22	C13H22N2O1	P-AMINOBENZYL,DIETHYLAMINOETHYL ETHER
4660	OLEYL ALCOHOL	459	31	2.32	2.89	C13H22N2O1	P-AMINOPHENYL,DIETHYLAMINOPROPYL ETHER
4661	OLEYL ALCOHOL	459	31	1.13	1.68	C13H22N2O2S1	P-AMINOPHENYL,DIETHYLAMINOPROPYL SULFONE
4662	OLEYL ALCOHOL	459	31	2.90	3.47	C13H22N2S1	ANILINE,4-DIETHYLAMINOPROPYLMERCAPTO
4663	OCTANOL	348		0.85	0.85 =	C13H23N1O2	N-OCTANOYLCYCLOBUTANECARBOXAMIDE
4664	CHCL3	424	46	-2.85		C13H26I1N1O2	1,2,2,6,6-PENTAMETHYL-4-ACETYL PIPERIDINE MEI
4665	CHCL3	424	46	-2.00		C13H26I1N1O2	1,3,3,5,5-PENTAMETHYL-4-ACETYL PIPERIDINE MEI
4666	DIETHYL ETHER	378	44	0.70	0.32 B	C13H26N2O2	N-CYCLOHEXYLCARBAMIC ACID,DIETAMINOETHYL ESTER
4667	OCTANOL	268	46	1.15	1.15 =	C13H29N3.C2H4O2	DODECYLGUANIDIUM ACETATE
4668	OCTANOL	268	46	1.00	1.00 =	C13H30BR1N3	DODECYLGUANIDINE HYDROBROMIDE
4669	OCTANOL	297	46	-0.16	-0.16 =	C13H30I1N1	TRIMETHYL-DECYL-AMMONIUM IODIDE
4670	CYCLOHEXANE	304		3.01		C14H8O2	ANTHROQUINONE
4671	CYCLOHEXANE	141		1.39		C14H8O2	PHENANTHRENEQUINONE
4672	DIETHYL ETHER	143	62	4.35	3.93 A	C14H8O3S1	2-HYDROXYNAPHTHOQUINONE,3-(W-A-THIENYLPROPYL)
4673	HEXANE	317		4.96		C14H9CL5	DDT
4674	OCTANOL	427		4.45	4.45 =	C14H10	ANTHRACENE
4675	OCTANOL	427		4.46	4.46 =	C14H10	PHENANTHRENE
4676	OILS	224		4.60	4.24 B	C14H10	PHENANTHRENE
4677	OCTANOL	463		2.69	2.69 =	C14H10O2	9-CARBOXYFLUORENE
4678	OCTANOL	463		2.46	2.46 =	C14H10O2S1	9-CARBOXYXTHIOXANTHENE
4679	OCTANOL	463		0.89	0.89 =	C14H10O3	9-CARBOXY-9-HYDROXYFLUORENE
4680	OCTANOL	463		2.12	2.12 =	C14H10O3	9-CARBOXYXANTHENE
4681	PARAFFINS	316		1.86		C14H11N1	9-AMINOPHENANTHRENE
4682	CYCLOHEXANE	141		4.40		C14H11N1O2	FLUORENE,9-NITROMETHYLENE
4683	CHCL3	464	46	4.96		C14H12N1.C10H21O4S1	N-METHYLACRIDINIUM DECYLSULFATE
4684	CHCL3	464	46	5.86		C14H12N1.C12H23O4S1	N-METHYLACRIDINIUM DODECYLSULFATE
4685	PARAFFINS	439		1.36		C14H12N2	9-AMINO-3-METHYLPHENANTHRIDINE
4686	OCTANOL	10		2.99	2.99 =	C14H12N2O3	PHENOXYACETIC ACID,4-PHENYLAZO
4687	CYCLOHEXANE	141		-2.31		C14H12N2O4	1,4-NAPHTHOQUINONE,2,3-DIACETAMIDO
4688	OCTANOL	235		3.97	3.97 =	C14H12O2	BENZYLBENZOATE
4689	OCTANOL	463		2.06	2.06 =	C14H12O2	A,A-DIPHENYLACETIC ACID
4690	DIETHYL ETHER	46		2.50	2.32 A	C14H12O3	BENZILIC ACID
4691	CHCL3	29		1.08	2.20 A	C14H12O3	BENZILIC ACID
4692	CHCL3	46		0.85	1.99 A	C14H12O3	BENZILIC ACID
4693	XYLENE	46		-0.04	1.74 A	C14H12O3	BENZILIC ACID
4694	TOLUENE	29		0.34	1.88 A	C14H12O3	BENZILIC ACID
4695	OCTANOL	10		3.18	3.18 =	C14H12O3	PHENOXYACETIC ACID,M-PHENYL
4696	OCTANOL	276		4.28	4.28 =	C14H12O3S1	2-OH-3-CARBOXYBENZTHIOPHENYL ETHER /PKA = 3.00/
4697	DIETHYL ETHER	465	62	2.70	2.49 A	C14H12O5	2-HYDROXYNAPHTHOQUINONE,3-(2-CARBOMETHOXYETHYL)
4698	OCTANOL	276		2.90	2.90 =	C14H13N1	DIHYDROMORPHANTHRIDINE /PKA = 3.00/
4699	N-HEPTANE	443		2.83		C14H13N1O2S1	PHENOTHIAZINE,3,7-DIMETHOXY
4700	N-HEPTANE	370	14	1.52		C14H13N1O3	P-AMINOSALICYLIC ACID,BENZYL ESTER

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4701	HEXANE	391		2.19		C14H13N103	N-METHYL CARBAMATE,N-ACETYL,1-NAPHTHYL
4702	N-HEPTANE	443		4.08		C14H13N1S1	PHENOTHIAZINE,3,7-OIMETHYL
47C3	OCTANOL	218		4.79	4.79 =	C14H14	8IBENZYL
4704	OCTANOL	276		4.82	4.82 =	C14H14	1,2-OIPHENYLETHANE
47C5	OCTANOL	65	46	-1.56	-1.56 =	C14H148R1N1	CINNAMYLPYRIOINIUM BROMIOE
47C6	CYCLOHEXANE	141		2.67		C14H148R1N102	1,4-NAPHTHOQUINONE,2-BROMO,3-BUTYLAMINO
47C7	OCTANOL	141		4.26	4.26 =	C14H14CL1N102	1,4-NAPHTHOQUINONE,2-CHLORO-3-BUTYLAMINO
47C8	CYCLOHEXANE	141		2.64		C14H14CL1N102	1,4-NAPHTHOQUINONE,2-CHLORO,3-BUTYLAMINO
4709	OCTANOL	235	77	-1.78	-1.78 =	C14H14CL1N3.HCL	ACRIFLAVINE HYOROCHLORIOE
4710	CHCL3	444	30	1.43	1.94 N	C14H14N203S1	N1-(3-ACETYLPHENYL)SULFANILAMIOE
4711	OCTANOL	141	26	3.29	3.29 =	C14H1402S1	1,4-NAPHTHOQUINONE, 2-BUTYLTHIO
4712	CYCLOHEXANE	141		3.43		C14H1402S1	1,4-NAPHTHOQUINONE,2-BUTYLTHIO
4713	OIETHYL ETHER	143	62	3.68	3.35 A	C14H1403	2-HYOROXYNAPHTHOQUINONE,3-BUTYL
4714	OIETHYL ETHER	143	62	3.60	3.27 A	C14H1403	2-HYOROXYNAPHTHOQUINONE,3-I-BUTYL
4715	OIETHYL ETHER	143	62	0.68	0.72 A	C14H1404	2-HYOROXYNAPHTHOQUINONE,3-(W-OIMETHYL-W-OH-ETHYL)
4716	CYCLOHEXANE	304		1.79		C14H1405	ETHYLACETOACETATE,3,4-METHYLENEOIOXYBENZAL
4717	CYCLOHEXANE	304		3.52		C14H15CL104	OIETHYLMALONATE,4-CHLOROBENZAL
4718	CYCLOHEXANE	304		3.28		C14H15F104	OIETHYLMALONATE,2-FLUOROBENZAL
4719	CYCLOHEXANE	304		3.32		C14H15F104	OIETHYLMALONATE,4-FLUOROBENZAL
4720	CYCLOHEXANE	304		3.82		C14H15F104	OIETHYLMALONATE,3-FLUOROBENZAL
4721	OIETHYL ETHER	466		2.77	2.43 A	C14H15N1	OIBENZYLAMINE
4722	CYCLOHEXANE	141		0.66		C14H15N1	OIBENZYLAMINE
4723	CHCL3	466		0.40	3.20 B	C14H15N1	OIBENZYLAMINE
4724	HEXANE	466		4.69		C14H15N1	OIBENZYLAMINE
4725	PARAFFINS	316		1.96		C14H15N1	4-OIMETHYLAMINOBIPHENYL
4726	PARAFFINS	316		3.19		C14H15N1	N-(4-OIPHENYL)-ETHYLAMINE
4727	PARAFFINS	316		0.42		C14H15N101	N-(4-OIPHENYL)-AMINOETHANOL
4728	OIETHYL ETHER	466		3.19	2.84 A	C14H15N101	2-HYDROXYIMINOOIBENZYL
4729	CHCL3	466		3.29	2.59 B	C14H15N101	2-HYOROXYIMINOOIBENZYL
4730	HEXANE	466		1.51		C14H15N101	2-HYOROXYIMINOOIBENZYL
4731	OCTANOL	141		3.11	3.11 =	C14H15N102	1,4-NAPHTHOQUINONE, 2-BUTYLAMINO
4732	CYCLOHEXANE	141		2.39		C14H15N102	1,4-NAPHTHOQUINONE,2-BUTYLAMINO
4733	CYCLOHEXANE	141		2.23		C14H15N102S1	1,4-NAPHTHOQUINONE,2-AMINO,3-BUTYLTHIO
4734	CYCLOHEXANE	304		2.50		C14H15N104	ETHYLCYANOACETATE,2,4-OIETHOXYBENZAL
4735	CYCLOHEXANE	304		2.20		C14H15N104	ETHYLCYANOACETATE,3,4-OIMETHOXYBENZAL
4736	CYCLOHEXANE	304		2.65		C14H15N104	ETHYLCYANOACETATE,3,5-OIMETHOXYBENZAL
4737	CYCLOHEXANE	304		2.26		C14H15N106	OIETHYLMALONATE,2-NITROBENZAL
4738	CYCLOHEXANE	304		2.71		C14H15N106	OIETHYLMALONATE,4-NITROBENZAL
4739	CYCLOHEXANE	304		2.81		C14H15N106	OIETHYLMALONATE,3-NITROBENZAL
4740	OCTANOL	302		4.58	4.58 =	C14H15N3	AZOBENZENE,4-OIMETHYLAMINO
4741	CHCL3	467		1.09	2.40 A	C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4742	BENZENE	467	7	0.10	1.50 A	C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4743	TOLUENE	467		-0.29	1.29 A	C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4744	NITROBENZENE	467		1.07	1.75	C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4745	N-BUTYL ACETATE	467		1.97	1.85	C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4746	CCL4	467		-1.13		C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4747	ME-1-BUT.KETONE	467	7	1.81	1.69	C14H1504P1	OIBENZYLPHOSPHORIC ACIO
4748	OCTANOL	65	46	-1.86	-1.86 =	C14H168R1N1	G-PHENYLPROPYLPYRIOINIUM BROMIOE
4749	OIETHYL ETHER	457	62	0.95	0.95 A	C14H16N202	1,4-NAPHTHOQUINONE,2-BUTYLHYORAZINO
4750	OIETHYL ETHER	457	62	0.87	0.88 A	C14H16N202	1,4-NAPHTHOQUINONE,2-I-BUTYLHYORAZINO
4751	OCTANOL	393	63	2.52	2.52 =	C14H16N202S1	N-SULFANILYL-3,4-XYLAMIOE
4752	CHCL3	393	63	2.08	2.54 N	C14H16N202S1	N-SULFANILYL-3,4-XYLAMIOE
4753	MIXEO SOLV#1	433		0.32		C14H16N205	BARBITURIC ACIO,1-CARBETHOXYMETHYL-5-5-OIALLYL
4754	OCTANOL	134		2.07	2.07 =	C14H16N402S1	3-BENZOYLMETHIO-4-AMINO-6-1-PR-1,2,4-TRIAZINE-5-ONE
4755	CYCLOHEXANE	304		2.35		C14H1603	ETHYLACETOACETATE,4-METHYLBENZAL
4756	CYCLOHEXANE	304		2.50		C14H1603	ETHYLACETOACETATE,3-METHYLBENZAL
4757	CYCLOHEXANE	304		2.58		C14H1603	ETHYLACETOACETATE,2-METHYLBENZAL
4758	CYCLOHEXANE	304		1.00		C14H1604	ACETYLACETONE,2,4-OIMETHOXYBENZYL
4759	CYCLOHEXANE	141		3.26		C14H1604	BENZALMALONATE,OIETHYL ESTER
4760	CYCLOHEXANE	304		1.91		C14H1604	ETHYLACETOACETATE,4-METHOXYBENZAL
4761	CYCLOHEXANE	304		1.93		C14H1604	ETHYLACETOACETATE,3-METHOXYBENZAL
4762	OCTANOL	65		2.97	2.97 =	C14H17F3N201	1-CYCLOBUTYL-1-ET-3-(M-TRIFLUOROMETHYLPHENYL)-UREA
4763	CYCLOHEXANE	446		0.82		C14H17N101	N-CYCLOPENTYLCINNAMAMIOE
4764	CYCLOHEXANE	446		1.44		C14H17N101	N,N-PENTAMETHYLENECINNAMAMIOE
4765	OCTANOL	227		-0.20	-0.20 =	C14H17N309	6-AZAURIOINE TRIACETATE (PKA=6.35)(NCS 67239)
4766	CHCL3	448	65	0.36		C14H18N202	N,N-OIMETHYLTRYPTAMINE, 5-ACETYL
4767	OILS	442		1.81	2.84 A	C14H18N203	METHOHEXITAL
4768	OCTANOL	10		3.79	3.79 =	C14H1803	PHENOXYACETIC ACIO,4-CYCLOHEXYL
4769	OLEYL ALCOHOL	142		1.53	2.08	C14H19N103	2-METHOXY-4-ALLYLPHENOXYACETAMIOE,N,N-OIMETHYL
4770	OILS	447		0.01	1.25 A	C14H208R1N101	A-BROMO-I-VALERYL-PSEUDOCUMIOINE
4771	N-HEPTANE	416	14	1.30		C14H20CL1N103	P-AMINOSALICYLIC ACIO,7-CHLOROHEPTYL ESTER
4772	N-HEPTANE	138		3.95		C14H20F3N1	N-BUTYLNORFENFLURAMINE
4773	CHCL3	448	65	0.27		C14H20N2	N,N-OIETHYLTRYPTAMINE
4774	CHCL3	448	65	0.76		C14H20N201	N-METHYL-N-ETHYLTRYPTAMINE, 5-METHOXY
4775	OCTANOL	56		4.83	4.83 =	C14H2003	P-HYOROXYBENZOIC ACIO,HEPTYL ESTER
4776	OCTANOL	438		0.26	0.26 =	C14H2006	GLUCOPYRANOSIOE,3,5-OIMETHYLPHENYL (BETA)
4777	OCTANOL	438		0.31	0.31 =	C14H2006	GLUCOPYRANOSIOE,3-ETHYLPHENYL (BETA)
4778	OLEYL ALCOHOL	390	44	4.26	4.80	C14H21N102	P-AMINOBENZOIC ACIO,HEPTYL ESTER
4779	HEXANE	391		2.48		C14H21N102	N-METHYL CARBAMATE,3,5-OI-I-PROPYLPHENYL
4780	N-HEPTANE	370	14	1.42		C14H21N103	P-AMINOSALICYLIC ACIO,N-HEPTYL ESTER
4781	N-HEPTANE	370	14	0.86		C14H21N104	P-AMINOSALICYLIC ACIO,7-HYOROXYHEPTYL ESTER
4782	OCTANOL	468		1.76	1.76 =	C14H21N302	1-(2-OIMEAMINOET)-3(M-MEOPHENYL)-2-IMIOAZOLIOINONE
4783	OLEYL ALCOHOL	459	31	2.44	3.01	C14H22N201	P-AMINOPHENYL,OIETHYLAMINOPROPYL KETONE
4784	OLEYL ALCOHOL	460		2.24	2.78	C14H22N202	P-AMINOBENZOIC ACIO,A-ME-B-(OIETAM)-ETHYL ESTER
4785	OLEYL ALCOHOL	460		2.32	2.86	C14H22N202	P-AMINOBENZOIC ACIO,B-ME-B-(OIETAM)ETHYL ESTER
4786	OCTANOL	449		3.15	3.15 =	C14H22N202	BENZOIC ACIO,P-PR-AMINO,N,N-OIMETHYLAMINOETHYL ESTER
4787	OILS	449		1.95	2.96 A	C14H22N202	BENZOIC ACIO,P-PR-AMINO,N,N-OIMETHYLAMINOETHYL ESTER
4788	XYLENE	449		2.81		C14H22N202	BENZOIC ACIO,P-PR-AMINO,N,N-OIMETHYLAMINOETHYL ESTER
4789	OI-BUTYL ETHER	449		2.25		C14H22N202	BENZOIC ACIO,P-PR-AMINO,N,N-OIMETHYLAMINOETHYL ESTER
4790	OIETHYL ETHER	378	44	0.78	1.62 B	C14H22N202	N-M-TOLYLCARBAMIC ACIO,OIETHYLAMINOETHYL ESTER
4791	OIETHYL ETHER	378	44	0.46	1.34 B	C14H22N202	N-O-TOLYLCARBAMIC ACIO,OIETHYLAMINOETHYL ESTER
4792	OIETHYL ETHER	378	44	0.75	1.60 B	C14H22N202	N-P-TOLYLCARBAMIC ACIO,OIETHYLAMINOETHYL ESTER
4793	OIETHYL ETHER	378	44	0.36	1.26 B	C14H22N203	N-M-METHOXYPHENYLCARBAMIC ACIO,OIETAMINOET.ESTER
4794	OIETHYL ETHER	378	44	0.55	1.42 B	C14H22N203	N-O-METHOXYPHENYLCARBAMIC ACIO,OIETAMINOET.ESTER
4795	OIETHYL ETHER	378	44	0.35	1.24 B	C14H22N203	N-P-METHOXYPHENYLCARBAMIC ACID,OIETAMINOET.ESTER
4796	OI-I-PR. KETONE	93	46	-0.58		C14H22N407	TETRAETHYLAMMONIUM PICRATE
4797	OCTANOL	373		-0.14	-0.14 =	C14H23CL1N201	N1-OCTYLNICOTINAMIOE CHLORIOE
4798	OLEYL ALCOHOL	459	31	3.26	3.83	C14H24N2	ANILINE,P-(4-OIETHYLAMINOBUTYL)
4799	OCTANOL	341	60	1.47	1.47 =	C14H24N2	N,N-OIBUTYL-3-PYRIOYLMETHYLAMINE
4800	N-HEPTANE	139	31	4.28		C14H2802	TETRAOECANOIC ACIO/MYRISTIC ACIO/

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4801	OCTANOL	297	46	-1.30	-1.30 =	C14H32I1N1	TRIBUTYLETHYLAMMONIUM IODIDE
4802	OCTANOL	409		2.90	2.90 =	C15H10O2	2-PHENYL-1,3-INDANEDIONE
4803	OCTANOL	469		2.36	2.36 =	C15H11CL1N2O1	QUINAZOLIN-2-ONE,1-ME-4-PHENYL-7-CHLORO
4804	OCTANOL	469		2.38	2.38 =	C15H11CL1N2O1	QUINAZOLIN-2-ONE,1-ME-4-PHENYL-6-CHLORO
4805	OCTANOL	469		1.87	1.87 =	C15H11F1N2O1	QUINAZOLIN-2-ONE,1-ME-4-PHENYL-6-FLUORO
4806	OCTANOL	469		1.79	1.79 =	C15H12N2O1	QUINAZOLIN-2-ONE
4807	OILS	470		1.96	2.97 A	C15H12N2O1S1	5,5-DIPHENYL-2-THIOHYDANTOIN
4808	OILS	470		0.96	2.06 A	C15H12N2O2	5,5-DIPHENYLHYDANTOIN
4809	OCTANOL	218		2.47	2.47 =	C15H12N2O2	HYDANTOIN, 5,5-DIPHENYL
4810	OCTANOL	469		1.72	1.72 =	C15H12N2O2	QUINAZOLIN-2-ONE,6-HYDROXY
4811	CYCLOHEXANE	141		3.94		C15H12O1	BENZALACETOPHENONE
4812	OCTANOL	463		2.67	2.67 =	C15H12O2	9-CARBOXY-9,10-DIHYDROANTHRACENE
4813	OCTANOL	276		4.69	4.69 =	C15H13CL1O3S1	2-OH-3-CARBOXY-5-ME-BENZTHIO-2'-CL-PHENYL ETHER
4814	CYCLOHEXANE	304		1.13		C15H13N1O1	CINNAMANILIDE
4815	CHCL3	471		3.18	3.61 N	C15H13N1O2	PHENYLHYDROXYLAMINE,N-CINNAMOYL
4816	OCTANOL	10		1.99	1.99 =	C15H13N1O4	PHENOXYACETIC ACID,3-BENZAMIDO
4817	CHCL3	306		1.70	2.69 A	C15H14I1N1O4S1	N-(P-IODOBENZENESULFONYL)PHENYLALANINE
4818	CCL4	306		-0.12	1.83 A	C15H14I1N1O4S1	N-(P-IODOBENZENESULFONYL)PHENYLALANINE
4819	PARAFFINS	439		2.35		C15H14N2	9-AMINO-1,3-DIMETHYLPHENANTHRIDINE
4820	OCTANOL	393	63	1.57	1.57 =	C15H14N4O2S1	SULFAPHENAZOLE
4821	CHCL3	343	2	1.41	1.93 N	C15H14N4O2S1	SULFAPHENAZOLE
4822	CHCL3	393	63	1.45	1.96 N	C15H14N4O2S1	SULFAPHENAZOLE
4823	BENZENE	343	2	0.64	1.95 A	C15H14N4O2S1	SULFAPHENAZOLE
4824	I-PENT. ACETATE	343	2	1.94	1.83	C15H14N4O2S1	SULFAPHENAZOLE
4825	CCL4	343	2	-0.83	1.15 A	C15H14N4O2S1	SULFAPHENAZOLE
4826	OCTANOL	463		2.58	2.58 =	C15H14O2	A,A-DIPHENYLPROPIONIC ACID
4827	DIETHYL ETHER	143	62	3.81	3.46 A	C15H14O3	2-HYDROXYNAPHTHOQUINONE,3-W-DIMETHYLALLYL
4828	DIETHYL ETHER	143	62	1.50	1.44 A	C15H14O4	2-HYDROXYNAPHTHOQUINONE,3-(W-DIMETHYLACETONYL)
4829	DIETHYL ETHER	143	62	1.33	1.29 A	C15H14O4	2-HYDROXYNAPHTHOQUINONE,3-(W-ME-W-HYDROXYME-ALLYL)
4830	DIETHYL ETHER	465	62	3.10	2.84 A	C15H14O5	2-HYDROXYNAPHTHOQUINONE,3-(3-CARBOMETHOXYPROPYL)
4831	DIETHYL ETHER	465	62	2.00	1.87 A	C15H14O5	2-HYDROXYNAPHTHOQUINONE,3-(4-CARBOXYBUTYL)
4832	OCTANOL	276		2.82	2.82 =	C15H15N1	DIBENZAZOCINE
4833	N-HEPTANE	370	14	2.01		C15H15N1O3	P-AMINOSALICYLIC ACID,B-PHENYLETHYL ESTER
4834	OILS	447		0.03	1.28 A	C15H16BR1N1O1	A-BROMO-I-VALERYL-A-NAPHTHYLAMINE
4835	DIETHYL ETHER	457	62	1.19	1.17 A	C15H16N2O2	1,4-NAPHTHOQUINONE,2-CYCLOPENTYLHYDRAZINO
4836	CYCLOHEXANE	141		2.93		C15H16N2O2	1-PHENYL-1-P-TOLUIDINO-2-NITROETHANE
4837	DIETHYL ETHER	3		0.70	1.46 B	C15H16N4	NEUTRAL RED BASE
4838	1-BUTANOL	4		2.04	2.36	C15H16N4	NEUTRAL RED BASE
4839	CHCL3	455		7.30		C15H16N4S1	THIOCARBAZONE,2,2-DIMETHYDIPHENYL
4840	CYCLOHEXANE	141		4.70		C15H16O2S1	1,4-NAPHTHOQUINONE,2-METHYL,3-BUTYLTHIO
4841	DIETHYL ETHER	143	62	4.27	3.87 A	C15H16O3	2-HYDROXYNAPHTHOQUINONE,3-I-PENTYL
4842	DIETHYL ETHER	143	62	1.58	1.51 A	C15H16O4	2-HYDROXYNAPHTHOQUINONE,3-(3-HYDROXYMETHYLBUTYL)
4843	DIETHYL ETHER	143	62	1.65	1.57 A	C15H16O4	2-HYDROXYNAPHTHOQUINONE,3-(2-HYDROXY-3-METHYLBUTYL)
4844	DIETHYL ETHER	143	62	1.24	1.21 A	C15H16O4	2-HYDROXYNAPHTHOQUINONE,3-(W-DIMETHYL-W-OH-PROPYL)
4845	PARAFFINS	316		-1.07		C15H17N1O2	3-(N-4-DIPHENYLAMINO)-PROPANE-1,2-DIOL
4846	CYCLOHEXANE	141		2.92		C15H17N1O2	1,4-NAPHTHOQUINONE,2-METHYL,3-BUTYLAMINO
4847	OCTANOL	283		-1.87	-1.87 =	C15H18BR1N1	P-BIPHENYLTRIMETHYLAMMONIUM BROMIDE
4848	DIETHYL ETHER	457	62	1.44	1.39 A	C15H18N2O2	1,4-NAPHTHOQUINONE,2-PENTYLHYDRAZINO
4849	CYCLOHEXANE	304		2.69		C15H18O1	ACETYLACETONE,2,4,6-TRIMETHYLBENZAL
4850	CYCLOHEXANE	304		4.00		C15H18O4	DIETHYLMALONATE,3-METHYLBENZAL
4851	CYCLOHEXANE	304		1.09		C15H18O4	ETHYLACETOACETATE,3,4-DIMETHOXYBENZAL
4852	CYCLOHEXANE	304		1.80		C15H18O4	ETHYLACETOACETATE,2,4-DIMETHOXYBENZAL
4853	CYCLOHEXANE	304		2.75		C15H18O4	ETHYLACETOACETATE,2,3-DIMETHOXYBENZAL
4854	CYCLOHEXANE	304		2.98		C15H18O5	DIETHYLMALONATE,4-METHOXYBENZAL
4855	CYCLOHEXANE	304		3.49		C15H18O5	DIETHYLMALONATE,2-METHOXYBENZAL
4856	CYCLOHEXANE	304		3.59		C15H18O5	DIETHYLMALONATE,3-METHOXYBENZAL
4857	CYCLOHEXANE	304		1.36		C15H18O6	DIETHYLMALONATE,3-METHOXY,4-HYDROXYBENZAL
4858	CYCLOHEXANE	446		1.39		C15H19N1O1	N-CYCLOHEXYLCINNAMAMIDE
4859	CYCLOHEXANE	446		1.97		C15H19N1O1	N,N-HEXAMETHYLENECINNAMAMIDE
4860	CCL4	472		1.76		C15H21AL1O6	ALUMINUM-TRI-ACETYLACETONATE
4861	CHCL3	472		3.64		C15H21CO1O6	COBALT TRI-ACETYLACETONATE
4862	BENZENE	472		2.04	2.18 B	C15H21CO1O6	COBALT TRI-ACETYLACETONATE
4863	CCL4	472		1.54		C15H21CO1O6	COBALT-TRI-ACETYLACETONATE
4864	CCL4	472		2.00		C15H21CR1O6	CHROMIUM-TRI-ACETYLACETONATE
4865	CHCL3	396	31	3.62	2.87 B	C15H21N1	FENCAMFAMINE
4866	N-HEPTANE	396	31	2.04		C15H21N1	FENCAMFAMINE
4867	OCTANOL	283		-1.54	-1.54 =	C15H21N1O1.HCL	2-METHYL-5-ET-2'-OH-6,7-BENZOMORPHAN/NIH#7910/
4868	OLEYL ALCOHOL	142		1.99	2.54	C15H21N1O2	4-ALLYLPHENOXYACETAMIDE,N,N-DIETHYL
4869	OCTANOL	9		0.17	0.17 =	C15H21N3O2	PHYSOSTIGMINE
4870	CCL4	472		2.04		C15H21RH1O6	RHENIUM-TR-ACETYLACETONATE
4871	N-HEPTANE	416	14	1.42		C15H22CL1N1O3	P-AMINOSALICYLIC ACID,B-CHLOROOCTYL ESTER
4872	CHCL3	448	65	0.90		C15H22N2O1	N,N-DIETHYLTRYPTAMINE, 5-METHOXY
4873	OCTANOL	438		0.65	0.65 =	C15H22O6	GLUCOPYRANOSIDE,3-ISOPROPYLPHENYL (BETA)
4874	OLEYL ALCOHOL	390	44	4.78	5.32	C15H23N1O2	P-AMINOBENZOIC ACID,OCTYL ESTER
4875	N-HEPTANE	370	14	1.48		C15H23N1O3	P-AMINOSALICYLIC ACID,N-OCTYL ESTER
4876	OLEYL ALCOHOL	473		3.54	4.11	C15H23N1O3	4-ETHOXYBENZOIC ACID,DIETHYLAMINOETHYL ESTER
4877	N-HEPTANE	370	14	1.01		C15H23N1O4	P-AMINOSALICYLIC ACID,B-HYDROXYOCTYL ESTER
4878	OCTANOL	218		0.55	0.55 =	C15H23N1O4	CYCLOHEXIMIDE
4879	OCTANOL	276		4.19	4.19 =	C15H23N3O2	2-(DIETAMINOME)-6-ME-7-NITROTETRAHYDROQUINOLINE /9.6/
4880	OLEYL ALCOHOL	460		2.78	3.32	C15H24N2O2	P-AMINOBENZOIC ACID,A,A-DIME-B-(DIETAM)-ETHYL ESTER
4881	OLEYL ALCOHOL	460		2.66	3.20	C15H24N2O2	P-AMINOBENZOIC ACID,A,B-DIME-B-(DIETAM)-ETHYL ESTER
4882	OLEYL ALCOHOL	460		2.57	3.11	C15H24N2O2	P-AMINOBENZOIC ACID,B,B-DIME-B-(DIETAM)ETHYL ESTER
4883	OCTANOL	449		3.73	3.73 =	C15H24N2O2	BENZOIC ACID,P-BU-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4884	DIETHYL ETHER	461		3.04	2.79 A	C15H24N2O2	BENZOIC ACID,P-BU-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4885	OILS	449		2.43	3.40 A	C15H24N2O2	BENZOIC ACID,P-BU-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4886	OILS	462		2.95	2.44 A	C15H24N2O2	BENZOIC ACID,P-BU-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4887	XYLENE	449		3.30		C15H24N2O2	BENZOIC ACID,P-BU-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4888	DI-BUTYL ETHER	449		2.76		C15H24N2O2	BENZOIC ACID,P-BU-AMINO,N,N-DIMETHYLAMINOETHYL ESTER
4889	DIETHYL ETHER	378	44	0.63	1.49 B	C15H24N2O2	N-2,4-DIMEPHENYLCARBAMIC ACID,DIETAMINOET.ESTER
4890	DIETHYL ETHER	378	44	0.78	1.62 B	C15H24N2O3	N-M-ETHOXYPHENYLCARBAMIC ACID,DIETAMINOET.ESTER
4891	DIETHYL ETHER	378	44	0.85	1.68 B	C15H24N2O3	N-O-ETHOXYPHENYLCARBAMIC ACID,DIETAMINOET.ESTER
4892	DIETHYL ETHER	378	44	0.78	1.62 B	C15H24N2O3	N-P-ETHOXYPHENYLCARBAMIC ACID,DIETAMINOET.ESTER
4893	CYCLOHEXANE	474	14	-0.07		C15H24N4O2S2	THIAMINE PROPYL DISULFIDE
4894	CHCL3	474	14	1.56	1.10 B	C15H24N4O2S2	THIAMINE PROPYL DISULFIDE
4895	BENZENE	474	14	-1.85		C15H24N4O2S2	THIAMINE PROPYL DISULFIDE
4896	ETHYL ACETATE	474	14	0.88	0.89	C15H24N4O2S2	THIAMINE PROPYL DISULFIDE
4897	OCTANOL	373		0.46	0.46 =	C15H25CL1N2O1	N1-NONYLNICOTINAMIDE CHLORIDE
4898	OCTANOL	65	46	-1.53	-1.53 =	C15H26BR1N1	BENZYLDIMETHYLHEXYLAMMONIUM BROMIDE
4899	OCTANOL	65	53	-0.72	-0.72 =	C15H26BR1N1	DECYLPYRIDINIUM BROMIDE
4900	DIETHYL ETHER	3	17	2.55	3.05 B	C15H26N2	SPARTEINE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
4901	1-BUTANOL	4		2.85	3.50	C15H26N2	SPARTEINE
4902	OCTANOL	56		2.54	2.54 =	C15H26O6	GLYCEROL, TRI-BUTYRATE
4903	OCTANOL	268	07	1.77	1.77 =	C15H32CL1N1	N-DECYLPIPERIDINE HYDROCHLORIDE
4904	CYCLOHEXANE	304		3.92		C16H9CL1O2	INDANE,1,3-DIONE,2(2-CHLOROBENZAL)
4905	CYCLOHEXANE	304		3.82		C16H9F1O2	INDANE,1,3-DIONE,2(2-FLUROBENZAL)
4906	CYCLOHEXANE	141		2.00		C16H10BR1N1O2	1,4-NAPHTHOQUINONE,2-BROMO,3-ANILINO
4907	OCTANOL	141		4.22	4.22 =	C16H10CL1N1O2	1,4-NAPHTHOQUINONE, 3-ANILINO-2-CHLORO
4908	CYCLOHEXANE	141		1.56		C16H10CL1N1O2	1,4-NAPHTHOQUINONE,2-CHLORO,3-ANILINO
4909	OCTANOL	141		-0.99	-0.99 =	C16H10K1N1O5S1	1,4-NAPHTHOQUINONE,2-ANILINO-3-SULFONATE,K-SALT
4910	CYCLOHEXANE	141		3.52		C16H10N2	BENZALMALONONITRILE,A-PHENYL
4911	CYCLOHEXANE	304		3.40		C16H10O2	INDANE,1,3-DIONE,2-BENZAL
4912	OCTANOL	141	26	4.40	4.40 =	C16H10O2	1,4-NAPHTHOQUINONE, 2-PHENYL
4913	CYCLOHEXANE	141		3.62		C16H10O2	1,4-NAPHTHOQUINONE,2-PHENYL
4914	CYCLOHEXANE	141		0.49		C16H10O3	1,4-NAPHTHOQUINONE,2-PHENYL,3-HYDROXY
4915	OCTANOL	141	26	2.14	2.14 =	C16H10O4S1	1,4-NAPHTHOQUINONE,2-PHENYLSULFONYL
4916	CYCLOHEXANE	141		1.50		C16H10O4S1	1,4-NAPHTHOQUINONE,2-PHENYLSULFONYL
4917	OCTANOL	469		2.69	2.69 =	C16H11F3N2O1	QUINAZOLIN-2-ONE,1-ME-4-PHENYL-6-TRIFLUOROMETHYL
4918	OCTANOL	141		2.84	2.84 =	C16H11N1O2	1,4-NAPHTHOQUINONE, 2-ANILINO
4919	CYCLOHEXANE	141		2.63		C16H11N1O2	1,4-NAPHTHOQUINONE,2-ANILINO
4920	CYCLOHEXANE	304		0.97		C16H11N1O3	COUMARIN,3-CARBOXYANILIDE
4921	N-HEPTANE	443		3.23		C16H11N1S1	PHENOTHIAZINE,3,4-BENZO
4922	N-HEPTANE	443		3.84		C16H11N1S1	PHENOTHIAZINE,1,2-BENZO
4923	OCTANOL	227		4.06	4.06 =	C16H12N2	5-METHYL-6H-PYRIDO(4,3-B)CARBAZOLE (87206)(PKA= 7.02)
4924	CYCLOHEXANE	304		2.11		C16H12N2O1	CYANOACETANILIDE,BENZAL
4925	CYCLOHEXANE	304		3.69		C16H12O1	1-INDANEONE,2-BENZYLIDINE
4926	OCTANOL	9		2.82	2.82 =	C16H13CL1N2O1	DIAZEPAM
4927	OCTANOL	218		2.44	2.44 =	C16H14CL1N3O1	LIBRIUM
4928	OCTANOL	469		1.91	1.91 =	C16H14N2O2	QUINAZOLIN-2-ONE,6-METHOXY
4929	OCTANOL	469		0.59	0.59 =	C16H14N2O3S1	QUINAZOLIN-2-ONE,1-ME-4-PHENYL-6-METHYLSULFONYL
4930	OCTANOL	276		2.58	2.58 =	C16H14O1	DIBENZOCYCLOOCTANE-5-ONE
4931	HEXANE	456		0.62		C16H15CL1O5	7-CL-4,6-DIMEO-6'-MEGRIS-2'-EN-3,4'-DIONE
4932	OCTANOL	276		2.33	2.33 =	C16H16	CYCLOPHANE
4933	DIETHYL ETHER	457	62	1.65	1.57 A	C16H16N2O2	1,4-NAPHTHOQUINONE,2-CYCLOHEXYLHYDRAZINO
4934	DIETHYL ETHER	457	62	1.64	1.56 A	C16H16N2O2	1,4-NAPHTHOQUINONE,2-CYCLOPENTYLMETHYLHYDRAZINO
4935	OCTANOL	56		-0.28	-0.28 =	C16H16N2O5S1	CEPHALOSPORANIC ACID,7-(D-MANDELAMIDO)-DESACETOXY
4936	N-HEPTANE	416	14	1.49		C16H16N2O6	BIS(P-AMINOSALICYLIC ACID) ETHYL ESTER
4937	DIETHYL ETHER	143	62	4.76	4.30 A	C16H16O3	2-HYDROXYNAPHTHOQUINONE,3-CYCLOHEXYL
4938	DIETHYL ETHER	465	62	2.40	2.23 A	C16H16O5	2-HYDROXYNAPHTHOQUINONE,3-(2-ME-3-CARBOMETHYOXYPROP
4939	DIETHYL ETHER	143	62	2.53	2.34 A	C16H16O5	2-HYDROXYNAPHTHOQUINONE,3-(W-CARBOMETHOXYBUTYL)
4940	DODECANE	475		4.45		C16H17CL1N2S1	ETHYL "CHLORPROMAZINE"
4941	N-HEPTANE	370	14	2.19		C16H17N1O3	P-AMINOSALICYLIC ACID,G-PHENYLPROPYL ESTER
4942	OCTANOL	141		2.07	2.07 =	C16H17N1O3S1	1,4-NAPHTHOQUINONE, 2-ACETAMIDO-3-BUTYLTHIO
4943	CYCLOHEXANE	141		1.28		C16H17N1O3S1	1,4-NAPHTHOQUINONE,2-ACETAMIDO,3-BUTYLTHIO
4944	CYCLOHEXANE	141		0.49		C16H18N2O3	1,4-NAPHTHOQUINONE,2-ACETAMIDO,3-BUTYLAMINO
4945	OCTANOL	127		1.83	1.83 =	C16H18N2O4S1	BENZYLPENICILLIN
4946	DIETHYL ETHER	106		1.93	1.82 A	C16H18N2O4S1	BENZYLPENICILLIN
4947	1-BUTANOL	130	12	0.20	-0.22	C16H18N2O4S1	BENZYLPENICILLIN
4948	ETHYL ACETATE	476		1.59	1.66	C16H18N2O4S1	BENZYLPENICILLIN
4949	N-BUTYL ACETATE	476		1.60	1.60	C16H18N2O4S1	BENZYLPENICILLIN
4950	OLEYL ALCOHOL	142		1.38	1.93	C16H18N2O5	MALONYL UREA,ETHYL-(2-MEO-4-ALLYLPHENOXY)
4951	OCTANOL	127		1.40	1.40 =	C16H18N2O5S1	PENICILLIN, A-HYDROXYBENZYL
4952	OCTANOL	127		2.09	2.09 =	C16H18N2O5S1	PHENOXYPENICILLIN/PENICILLIN V/
4953	1-BUTANOL	130		0.12	-0.34	C16H18N2O5S1	PHENOXYPENICILLIN/PENICILLIN V/
4954	OCTANOL	283	65	0.87	0.87 =	C16H18N4O2	NIALAMIDE
4955	DIETHYL ETHER	143	62	4.90	4.41 A	C16H18O3	2-HYDROXYNAPHTHOQUINONE,3-HEXYL
4956	OCTANOL	438		0.76	0.76 =	C16H18O6	GLUCOPYRANOSIDE,2-NAPHTHYL (BETA)
4957	HEXANE	456		-0.41		C16H19CL1O4	7-CL-6'-OH-4,6-DIMETHOXY-2'-MEGRISAN-3-ONE
4958	HEXANE	456		-2.82		C16H19CL1O5	7-CL-4',6'-DI-OH-4,6-DIMEO-2'-METHYLGRISAN-3-ONE
4959	CHCL3	396	31	3.35	2.64 B	C16H19N1	BENZYLAMPHETAMINE
4960	N-HEPTANE	396	31	2.04		C16H19N1	BENZYLAMPHETAMINE
4961	PARAFFINS	316		-0.58		C16H19N1O2	N,N-DI-B-HYDROXYETHYL-4-AMINOBIPHENYL
4962	CYCLOHEXANE	304		3.79		C16H19N1O3	ETHYLCYANOACETATE,3-BUTOXYBENZAL
4963	1-BUTANOL	130		-0.23	-0.83	C16H19N3O4S1	AMPICILLIN
4964	CYCLOHEXANE	304		3.35		C16H20O5	DIETHYLMALONATE,3-ETHOXYBENZAL
4965	CYCLOHEXANE	304		2.33		C16H20O6	DIETHYLMALONATE,3,4-DIMETHOXYBENZAL
4966	CYCLOHEXANE	304		3.22		C16H20O6	DIETHYLMALONATE,3,5-DIMETHOXYBENZAL
4967	OCTANOL	206		4.38	4.38 =	C16H21F3N2	BENZIMIDAZOLE,5-OCTYL-2-(TRIFLUOROMETHYL)
4968	CYCLOHEXANE	446		2.04		C16H21N1O1	N-CYCLOHEPTYLCINNAMAMIDE
4969	CYCLOHEXANE	446		2.46		C16H21N1O1	N,N-HEPTAMETHYLENECINNAMAMIDE
4970	CHCL3	405	31	2.86	2.21 B	C16H21N1O3	HOMATROPINE
4971	N-HEPTANE	477		-3.00		C16H21N1O3	HOMATROPINE
4972	OLEYL ALCOHOL	142		1.20	1.75	C16H21N1O4	2-METHOXY-4-ALLYLPHENOXYACETYLMORPHOLINE
4973	BENZENE	137		1.46	2.81	C16H22N1O2	2-ME-5-PH-5-CARBETHOXY-2-AZABICYC(2,2,1)HEPTANE/EXO/
4974	BENZENE	137		1.46	2.81	C16H22N1O2	2-ME-5-PH-5-CARBETHOXY-2-AZABICYC(2,2,1)HEPTANE/ENDO/
4975	DIETHYL ETHER	3		1.21	1.17 A	C16H22O11	GLUCOSE PENTA-ACETATE
4976	BENZENE	405	31	2.19	2.07 B	C16H23CL1N2O2	2-ALLYLOXYL-4-CL-N(2-DIETAMINOET)-BENZAMIDE
4977	OCTANOL	283		-1.31	-1.31 =	C16H23N1O1.HCL	2,9-DIMETHYL-5-ET-2'-OH-6,7-BENZOMORPHAN/NIH#7938
4978	OCTANOL	283		-1.52	-1.52 =	C16H23N1O1.HCL	2,5-DIMETHYL-9-ET-2'-OH-6,7-BENZOMORPHAN/NIH#7951
4979	CYCLOHEXANE	446		2.72		C16H23N1O1	N-HEPTYLCINNAMAMIDE
4980	OLEYL ALCOHOL	142		1.46	2.01	C16H23N1O2	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N-ME-N-PROPYL
4981	OLEYL ALCOHOL	142		2.51	3.05	C16H23N1O3	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N,N-DIETHYL
4982	OLEYL ALCOHOL	142		1.82	2.37	C16H23N1O3	2-METHOXY-6-ALLYLPHENOXYACETAMIDE,N,N-DIETHYL
4983	MIXED SOLV#1	433		2.28		C16H23N3O4	BARBITURIC ACID,1-(N,N-DIET-CARBAMYLME)-5,5-DIALLYL
4984	N-HEPTANE	416	14	1.48		C16H24CL1N1O3	P-AMINOSALICYLIC ACID,9-CHLORONONYL ESTER
4985	OLEYL ALCOHOL	142		0.55	1.01	C16H24N1O5	2-METHOXY-4-ETHOXYCARBONYLPHENOXYACETAMIDE,N,N-DIET
4986	OCTANOL	438		1.07	1.07 =	C16H24O6	GLUCOPYRANOSIDE,2-ISOPROPYL-5-MEPHENYL(BETA)
4987	OCTANOL	438		1.01	1.01 =	C16H24O6	GLUCOPYRANOSIDE,3-T-BUTYLPHENYL (BETA)
4988	N-HEPTANE	370	14	1.76		C16H25N1O3	P-AMINOSALICYLIC ACID,N-NONYL ESTER
4989	OLEYL ALCOHOL	142		2.70	3.24	C16H25N1O3	2-METHOXY-4-PROPYLPHENOXYACETAMIDE,N,N-DIETHYL
4990	N-HEPTANE	370	14	1.15		C16H25N1O4	P-AMINOSALICYLIC ACID,9-HYDROXYNONYL ESTER
4991	OLEYL ALCOHOL	473		2.81	3.38	C16H25N1O4	3-MEO-4-ETO-BENZOIC ACID,DIETHYLAMINOETHYL ESTER
4992	OLEYL ALCOHOL	473		2.39	2.96	C16H25N1O5	3,4,5-TRIMETHOXYBENZOIC ACID,DIETHYLAMINOETHYL ESTER
4993	OLEYL ALCOHOL	460		3.43	3.96	C16H26N2O2	P-AMINOBENZOIC ACID,A,A,B-TRIME-B-(DIETAM)-ETHYL EST.
4994	OLEYL ALCOHOL	460		3.48	4.04	C16H26N2O2	P-AMINOBENZOIC ACID,A,B,B-TRIME-B-(DIETAM)-ETHYL EST.
4995	OCTANOL	449		4.14	4.14 =	C16H26N2O2	BENZOIC ACID,P-AMYLAMINO,N,N-DIMEAMINOETHYL ESTER
4996	OILS	449		2.79	3.72 A	C16H26N2O2	BENZOIC ACID,P-AMYLAMINO,N,N-DIMEAMINOETHYL ESTER
4997	XYLENE	449		3.92		C16H26N2O2	BENZOIC ACID,P-AMYLAMINO,N,N-DIMEAMINOETHYL ESTER
4998	DI-BUTYL ETHER	449		3.33		C16H26N2O2	BENZOIC ACID,P-AMYLAMINO,N,N-DIMEAMINOETHYL ESTER
4999	OCTANOL	373		1.12	1.12 =	C16H27CL1N2O1	N1-DECYLNICOTINAMIDE CHLORIDE
5000	BENZENE	478		-1.52	-0.51 B	C16H32N2O1	PIPERIDINE,1-DECYL,3-CARBAMYL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5001	N-HEPTANE	479	31	5.31		C16H32O2	HEXADECANOIC ACID/PALMITIC ACID/
5002	DIETHYL ETHER	236	17	2.88		C16H34O4P1	DIOCTYLPHOSPHATE
5003	ME-1-BUT.KETONE	236	17	2.03	1.81	C16H35O4P1	DIOCTYLPHOSPHATE
5004	BENZENE	480		0.11	1.51 A	C16H35O4P1	PHOSPHORIC ACID,DI(2-ETHYLHEXYL)
5005	CCL4	480		0.09		C16H35O4P1	PHOSPHORIC ACID,DI(2-ETHYLHEXYL)
5006	NITROBENZENE	92	46	0.07		C16H36I1N1	TETRA-(N-BUTYL) AMMONIUM IODIDE
5007	OCTANOL	268		-1.00	-1.00 =	C16H38BR2N2	DECAMETHONIUM BROMIDE
5008	CYCLOHEXANE	141		4.22		C17H12CL1N1O2	1,4-NAPHTHOQUINONE,2-CL,3-ANILINO,6-METHYL
5009	CYCLOHEXANE	304		3.83		C17H12O2	INDANE,1,3-DIONE,2(2-METHYLBENZAL)
5010	CYCLOHEXANE	141		3.52		C17H12O2	1,4-NAPHTHOQUINONE,2-METHYL,3-PHENYL
5011	DIETHYL ETHER	143	62	3.16	2.89 A	C17H12O3	2-HYDROXYNAPHTHOQUINONE,3-PHENYLMETHYL
5012	CYCLOHEXANE	304		3.44		C17H12O3	INDANE,1,3-DIONE,2(2-METHOXYBENZAL)
5013	CYCLOHEXANE	141		3.05		C17H13N1O2	1,4-NAPHTHOQUINONE,2-ANILINO,6-METHYL
5014	CYCLOHEXANE	141		4.22		C17H13N1O2	1,4-NAPHTHOQUINONE,2-METHYL,3-ANILINO
5015	PRIM. PENTANOLS	481		2.34	2.62	C17H14N2O2	5-PYRAZOLONE,1-PHENYL,3-METHYL,4-BENZOYL
5016	DIETHYL ETHER	143	62	4.35	3.93 A	C17H14O3S1	2-HYDROXYNAPHTHOQUINONE,3-(W-A-THIENYLPROPYL)
5017	HEXANE	456		0.14		C17H17CL1O6	7-CL-4,6,4'-TRIMEO-6'-MEGRIS-3'-EN-3,2'-DIONE
5018	HEXANE	456		-0.10		C17H17CL1O6	DD-7-CL-4,6,2'-TRIMEO-6'-MEGRIS-2'-EN-3,4'-DIONE
5019	OCTANOL	238		2.18	2.18 =	C17H17CL1O6	GRISEOFULVIN
5020	HEXANE	456		0.26		C17H17CL1O6	LD-7-CL-4,6,2'-TRIMEO-6'-MEGRIS-2'-EN-3,4'-DIONE
5021	N-HEPTANE	416	14	1.62		C17H18N2O6	BIS(P-AMINOSALICYLIC ACID) PROPYL ESTER
5022	DIETHYL ETHER	143	62	4.93	4.44 A	C17H18O3	2-HYDROXYNAPHTHOQUINONE,3-CYCLOHEXYLMETHYL
5023	DIETHYL ETHER	465	62	3.70	3.36 A	C17H18O5	2-HYDROXYNAPHTHOQUINONE,3-(4-CARBOMETHOXYPENTYL)
5024	HEXANE	456		-0.44		C17H18O6	4,6,2'-TRIMEO-6'-MEGRIS-2'-EN-3,4'DIONE
5025	CHCL3	482	68	-1.05	-0.37 N	C17H19CL1N2O1S1	CHLORPROMAZINE SULFOXIDE
5026	DODECANE	475		-0.12		C17H19CL1N2O1S1	CHLORPROMAZINE-SULFOXIDE
5027	OCTANOL	475	46	-0.66	-0.66 =	C17H19CL1N2O1S1.HCL	CHLORPROMAZINE-SULFOXIDE.HCL
5028	OCTANOL	483	44	5.16	5.16 =	C17H19CL1N2S1	CHLORPROMAZINE
5029	OCTANOL	218		5.35	5.35 =	C17H19CL1N2S1	CHLORPROMAZINE
5030	OCTANOL	56		5.32	5.32 =	C17H19CL1N2S1	CHLORPROMAZINE
5031	CYCLOHEXANE	484		0.95		C17H19CL1N2S1	CHLORPROMAZINE
5032	CHCL3	482	68	1.09	1.62 N	C17H19CL1N2S1	CHLORPROMAZINE
5033	CHCL3	482	69	2.10	2.55 N	C17H19CL1N2S1	CHLORPROMAZINE
5034	N-HEPTANE	485	14	1.86		C17H19CL1N2S1	CHLORPROMAZINE
5035	DODECANE	475		4.86		C17H19CL1N2S1	CHLORPROMAZINE
5036	OCTANOL	475	46	1.51	1.51 =	C17H19CL1N2S1.HCL	CHLORPROMAZINE HYDROCHLORIDE
5037	CHCL3	486	46	1.22	1.73 N	C17H19CL1N2S1.HCL	CHLORPROMAZINE HYDROCHLORIDE
5038	OCTANOL	475	46	1.23	1.23 =	C17H19CL1N2S1.HCL	1-CHLORPROMAZINE HYDROCHLORIDE
5039	OCTANOL	475	46	1.79	1.79 =	C17H19CL1N2S1.HCL	3-CHLORPROMAZINE HYDROCHLORIDE
5040	DODECANE	475		4.79		C17H19CL1N2S1	1-CHLORPROMAZINE
5041	DODECANE	475		4.67		C17H19CL1N2S1	3-CHLORPROMAZINE
5042	OCTANOL	186		0.76	0.76 =	C17H19N1O3	MORPHINE
5043	OCTANOL	218		0.70	0.70 =	C17H19N1O3	MORPHINE
5044	DIETHYL ETHER	3	17	-0.68	0.25 B	C17H19N1O3	MORPHINE
5045	I-BUTANOL	4		0.87	0.72	C17H19N1O3	MORPHINE
5046	CHCL3	466		4.04	3.22 B	C17H20N2	DESDIMETHYLIMIPRAMINE
5047	HEXANE	466		2.38		C17H20N2	DESDIMETHYLIMIPRAMINE
5048	DIETHYL ETHER	457	62	2.03	1.89 A	C17H20N2O2	1,4-NAPHTHOQUINONE,2-CYCLOHEXYLMETHYLHYDRAZINO
5049	DIETHYL ETHER	457	62	2.13	1.99 A	C17H20N2O2	1,4-NAPHTHOQUINONE,2-W-CYCLOPENTYLETHYLHYDRAZINO
5050	N-HEPTANE	477		-1.70		C17H20N2O2	TROPIC ACID,N-ET-N-G-PICOLYLAMIDE
5051	OCTANOL	127		2.28	2.28 =	C17H20N2O5S1	PENICILLIN,A-PHENOXYETHYL
5052	1-BUTANOL	130		0.46	0.14	C17H20N2O5S1	PENICILLIN,A-PHENOXYETHYL
5053	OCTANOL	127		1.22	1.22 =	C17H20N2O6S1	PENICILLIN,2,6-DIMETHOXYPHENYL
5054	OCTANOL	483	44	4.55	4.55 =	C17H20N2S1	PROMAZINE
5055	CHCL3	482	68	0.59	1.16 N	C17H20N2S1	PROMAZINE
5056	CHCL3	482	69	1.43	1.94 N	C17H20N2S1	PROMAZINE
5057	N-HEPTANE	485	14	1.71		C17H20N2S1	PROMAZINE
5058	DODECANE	475		4.02		C17H20N2S1	PROMAZINE
5059	CYCLOHEXANE	484		1.50		C17H20N2S1	PROMETHAZINE
5060	CHCL3	482	68	-1.22	-0.53 N	C17H20N2S1	PROMETHAZINE
5061	CHCL3	482	69	1.76	2.25 N	C17H20N2S1	PROMETHAZINE
5062	DIETHYL ETHER	487		-3.80		C17H20N4O6	RIBOFLAVIN
5063	N-BUTANOL	487		-0.17	-0.75	C17H20N4O6	RIBOFLAVIN
5064	1-BUTANOL	487		-0.33	-0.97	C17H20N4O6	RIBOFLAVIN
5065	PRIM. PENTANOLS	487		-0.77	-1.28	C17H20N4O6	RIBOFLAVIN
5066	HEXANOL	487		-0.92	-1.25	C17H20N4O6	RIBOFLAVIN
5067	CYCLOHEXANOL	487		-0.27	-1.46	C17H20N4O6	RIBOFLAVIN
5068	PARAFFINS	487		-4.70		C17H20N4O6	RIBOFLAVIN
5069	DIETHYL ETHER	143	62	5.65	5.06 A	C17H20O3	2-HYDROXYNAPHTHOQUINONE,3-1-HEPTYL
5070	DIETHYL ETHER	465	62	2.24	2.09 A	C17H20O4	2-HYDROXYNAPHTHOQUINONE,3-(5-OH-5-METHYLHEXYL)
5071	OCTANOL	475	46	0.91	0.91 =	C17H21CL1N2S1	PROMAZINE HYDROCHLORIDE
5072	CHCL3	486	46	0.73	1.25 N	C17H21CL1N2S1	PROMAZINE HYDROCHLORIDE
5073	CHCL3	396	31	3.15	2.47 B	C17H21N1	BENZPHETAMINE
5074	N-HEPTANE	396	31	1.87		C17H21N1	BENZPHETAMINE
5075	OCTANOL	276		3.30	3.30 =	C17H21N1O1	BENADRYL /PKA= 8.98/
5076	OCTANOL	218		3.27	3.27 =	C17H21N1O1	DIPHENHYDRAMINE
5077	OCTANOL	218		3.40	3.40 =	C17H21N1O1	DIPHENHYDRAMINE
5078	N-HEPTANE	477		1.26		C17H21N1O1	DIPHENHYDRAMINE
5079	DIETHYL ETHER	3	17	2.14	2.73 B	C17H21N1O4	COCAINE
5080	OILS	462		2.33	1.92 B	C17H21N1O4	COCAINE
5081	1-BUTANOL	4		2.03	2.34	C17H21N1O4	COCAINE
5082	N-HEPTANE	477		-2.36		C17H21N1O4	SCOPOLAMINE
5083	DIETHYL ETHER	457	62	2.86	2.63 A	C17H22N2O2	1,4-NAPHTHOQUINONE,2-HEPTYLHYDRAZINO
5084	CYCLOHEXANE	304		4.00		C17H22O5	DIETHYLMALONATE,3-PROPOXYBENZAL
5085	CYCLOHEXANE	446		2.48		C17H23N1O1	N-CYCLOOCTYLCINNAMAMIDE
5086	CYCLOHEXANE	446		3.11		C17H23N1O1	N,N-OCTAMETHYLENECINNAMAMIDE
5087	OCTANOL	218		1.79	1.79 =	C17H23N1O3	ATROPINE
5088	OCTANOL	218		1.83	1.83 =	C17H23N1O3	ATROPINE
5089	DIETHYL ETHER	3	17	0.61	1.39 B	C17H23N1O3	ATROPINE
5090	1-BUTANOL	4	12	1.94	2.22	C17H23N1O3	ATROPINE
5091	DI-I-PR. ETHER	488		-0.03		C17H23N1O3	ATROPINE
5092	N-HEPTANE	477		-3.25		C17H23N1O3	ATROPINE
5093	OLEYL ALCOHOL	142		2.20	2.74	C17H23N1O3	2-METHOXY-4-ALLYLPHENOXYACETYLPIPERIDINE
5094	OCTANOL	276		2.85	2.85 =	C17H23N3O1	MEPYRAMINE / PKA = 8.85/
5095	OLEYL ALCOHOL	489	27	2.15	2.70	C17H23N3O2	CINCHONINAMIDE,N-(2-DIETHYL-AMINOETHYL)-2-METHOXY
5096	N-HEPTANE	477		-2.89		C17H24N2O2	ATURBAN
5097	CHCL3	490	17	0.33	0.05 B	C17H25CL1N2O1.HBR	1-(M-CLBENZYL)-3-N-DIETCARBAMOYL)PIPERIDIN
5098	CHCL3	490	17	0.40	0.11 B	C17H25CL1N2O1.HBR	1-(P-CLBENZYL)-3-N-DIETCARBAMOYL)PIPERIDIN
5099	CYCLOHEXANE	446		3.21		C17H25N1O1	N-OCTYLCINNAMAMIDE
5100	OLEYL ALCOHOL	142		2.97	3.51	C17H25N1O3	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N-ME,N-BUTYL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5101	OLEYL ALCOHOL	142		2.75	3.29	C17H25N1O3	2-METHOXY-4-ALLYLPHENOXYPROPIONAMIOE,N,N-OIETHYL
5102	CHCL3	491	46	-1.62		C17H25N1O7S1	ATROPINE SULFATE
5103	CHCL3	490	17	-0.12	-0.12 B	C17H25N3O3.HBR	1-(M-NO2BENZYL)-3-(N-OIETCARBAMOYL)PIPERIOINE
5104	CHCL3	490	17	0.00	-0.23 B	C17H25N3O3.HBR	1-(P-NO2BENZYL)-3-(N-OIETCARBAMOYL)PIPERIOINE
5105	N-HEPTANE	416	14	1.68		C17H26CL1N1O3	P-AMINOSALICYLIC ACIO,10-CHLOROOECYL ESTER
5106	CHCL3	490	17	-0.02	-0.25 B	C17H26N2O1.HBR	1-BENZYL-3-(N,N-OIETCARBAMOYL)PIPERIOINE-HBR
5107	MIXEO SOLV#I	433		2.23		C17H26N2O3	BARBITURIC ACIO,1-N-HEPTYL-5,5-OIALLYL
5108	CYCLOHEXANE	474	14	-0.77		C17H26N4O3S2	THIAMINE TETRAHYOROFURFURYL OISULFIOE
5109	CHCL3	474	14	1.17	0.77 B	C17H26N4O3S2	THIAMINE TETRAHYOROFURFURYL OISULFIOE
5110	BENZENE	474	14	-2.52		C17H26N4O3S2	THIAMINE TETRAHYOROFURFURYL OISULFIOE
5111	ETHYL ACETATE	474	14	0.07	0.06	C17H26N4O3S2	THIAMINE TETRAHYOROFURFURYL DISULFIOE
5112	N-HEPTANE	370	14	2.08		C17H27N1O3	P-AMINOSALICYLIC ACIO, OECYL ESTER
5113	OLEYL ALCOHOL	473		4.27	4.84	C17H27N1O3	4-BUTOXYBENZOIC ACIO,OIETHYLAMINOETHYL ESTER
5114	N-HEPTANE	370	14	1.24		C17H27N1O4	P-AMINOSALICYLIC ACIO,10-HYOROXYOECYL ESTER
5115	OLEYL ALCOHOL	473		3.52	4.09	C17H27N1O4	2,4-OIETHOXYBENZOIC ACIO,DIETHYLAMINOETHYL ESTER
5116	OLEYL ALCOHOL	473		3.37	3.90	C17H27N1O4	3,4-OIETHOXYBENZOIC ACIO,OIETHYLAMINOETHYL ESTER
5117	OLEYL ALCOHOL	460		3.29	3.82	C17H28N2O2	P-AMINOBENZOIC ACIO,TETRAME-B-(OIETAM(-ETHYL ESTER
5118	OIETHYL ETHER	378	44	1.10	1.90 B	C17H28N2O3	N-M-BUTOXYPHENYLCARBAMIC ACID,OIETAMINOET.ESTER
5119	OIETHYL ETHER	378	44	1.09	1.89 B	C17H28N2O3	N-O-BUTOXYPHENYLCARBAMIC ACIO,OIETAMINOET.ESTER
5120	OIETHYL ETHER	378	44	1.07	2.00 B	C17H28N2O3	N-P-BUTOXYPHENYLCARBAMIC ACIO,OIETAMINOET.ESTER
5121	CHCL3	464	46	2.70		C17H29N1O6S1	N-ME-3-METHOXYCARBONYLPYRIOINIUM NONYLSULFATE
5122	OCTANOL	65	46	-0.29	-0.29 =	C17H30BR1N1	BENZYLOIMETHYLOCTYLAMMONIUM BROMIOE
5123	OCTANOL	65	46	0.44	0.44 =	C17H30BR1N1	OOOECYLPYRIOINIUM BROMIOE
5124	OCTANOL	348		1.28	1.28 =	C17H31N1O2	N-DOOECANOYLCYCLOBUTANECARBOXAMIOE
5125	BENZENE	478		-1.15	-0.25 B	C17H34N2O1	PIPERIOINE,1-OECYL,3-(N-METHYLCARBAMYL)
5126	OCTANOL	297	46	-0.22	-0.22 =	C17H38I1N1	TRIPENTYL-ETHYL-AMMONIUM IODIOE
5127	CCL4	412		2.05		C18H12CU1N2O2	8-QUINOLINOLO(BIS)-CU(II)
5128	CHCL3	412		3.48		C18H12CU1N2O3	8-QUINOLINOLO(BIS)-CU(II)
5129	OCTANOL	141		1.73	1.73 =	C18H14N2O3	1,4-NAPHTHOQUINONE, 2-ACETAMIOO-3-ANILINO
5130	CYCLOHEXANE	141		-0.71		C18H14N2O3	1,4-NAPHTHOQUINONE,2-ACETAMIOO,3-ANILINO
5131	DIETHYL ETHER	143	62	4.04	3.68 A	C18H14O3	2-HYOROXYNAPHTHOQUINONE,3-(W-PHENYLETHYL)
5132	CHCL3	96		-0.42		C18H15BR1O3S1	TRIPHENYLSULFONIUM BROMATE
5133	CHCL3	96		-0.25		C18H15BR1S1	TRIPHENYLSULFONIUM BROMIOE
5134	CHCL3	96		-0.63		C18H15CL1S1	TRIPHENYLSULFONIUM CHLORIOE
5135	CHCL3	96		-2.52		C18H15I1O3S1	TRIPHENYLSULFONIUM IOOATE
5136	CHCL3	96		1.12		C18H15I1S1	TRIPHENYLSULFONIUM IOOIDE
5137	CHCL3	96		-1.00		C18H15N1O2S1	TRIPHENYLSULFONIUM NITRITE
5138	CHCL3	96		-0.29		C18H15N1O3S1	TRIPHENYLSULFONIUM NITRATE
5139	OCTANOL	56		2.87	2.87 =	C18H15O1P1	PHOSPHINE OXIOE,TRIPHENYL
5140	CHCL3	96	32	1.01		C18H17CR1O4S1	TRIPHENYLSULFONIUM CHROMATE
5141	CHCL3	96	33	-0.15		C18H17CR1O4S1	TRIPHENYLSULFONIUM CHROMATE
5142	CHCL3	96		-1.00		C18H17O4P1S1	TRIPHENYLSULFONIUM PHOSPHATE
5143	OCTANOL	56		-0.89	-0.89 =	C18H18N2O7S1	CEPHALOSPORANIC ACIO,7(O-MANOELAMIOO)
5144	HEXANE	456		0.36		C18H19CL1O6	7-CL-2'-ETO-4,6-OIMEO-6'-MEGRIS-2'-EN-3,4'-OIONE
5145	HEXANE	456		0.57		C18H19CL1O6	7-CL-4'-ETO-4,6-OIMEO-6'-MEGRIS-3'-EN-3,2'-OIONE
5146	OCTANOL	483	44	5.19	5.19 =	C18H19F3N2S1	TRIFLUPROMAZINE
5147	CHCL3	482	68	1.30	1.82 N	C18H19F3N2S1	TRIFLUPROMAZINE
5148	CHCL3	482	69	1.76	2.25 N	C18H19F3N2S1	TRIFLUPROMAZINE
5149	N-HEPTANE	485	14	1.15		C18H19F3N2S1	TRIFLUPROMAZINE
5150	OOOECANE	475		5.14		C18H19F3N2S1	TRIFLUPROMAZINE
5151	MIXEO SOLV#1	433		0.30		C18H19N3O4	BARBITURIC ACIO,1-(N-PHENYLCARBAMYLME)-5,5-DIALLYL
5152	OCTANOL	475	46	1.78	1.78 =	C18H20CL1F3N2S1	TRIFLUPROMAZINE HYOROCHLORIOE
5153	CHCL3	486	46	1.46	1.92 N	C18H20CL1F3N2S1	TRIFLUPROMAZINE HYOROCHLORIOE
5154	MIXEO SOLV#1	433		2.36		C18H20N2O3	BARBITURIC ACID,1-B-PHENYLETHYL-5,5-OIALLYL
5155	N-HEPTANE	416	14	1.74		C18H20N2O6	BIS(P-AMINOSALICYLIC ACIO) BUTYL ESTER
5156	CHCL3	482	68	0.88	1.43 N	C18H20N2S1	METHOILAZINE
5157	CHCL3	482	69	1.92	2.40 N	C18H20N2S1	METHOILAZINE
5158	CHCL3	482	68	1.14	1.67 N	C18H20N2S1	PYRATHIAZINE
5159	CHCL3	482	69	1.88	2.36 N	C18H20N2S1	PYRATHIAZINE
5160	OCTANOL	218		5.07	5.07 =	C18H20O2	4,4'-STILBENEOIOL,A,A'-OIETHYL
5161	OIETHYL ETHER	143	62	5.64	5.06 A	C18H20O3	2-HYOROXYNAPHTHOQUINONE,3-(W-CYCLOHEXYLETHYL)
5162	OCTANOL	276		4.36	4.36 =	C18H20O3S1	2-OH-3-CARBOXY-5-ME-BENZTHIO-2'-1-PROPYLPHENYLETHER
5163	OCTANOL	276		4.91	4.91 =	C18H20O4	2-OH-3-CARBOXY-5-ME-BENZYL-2'-1-PROPYLPHENYLETHER
5164	OIETHYL ETHER	465	62	3.40	3.10 A	C18H20O5	2-HYOROXYNAPHTHOQUINONE,3-(2-ME-5-CARBOMETHOXYPENT)
5165	OIETHYL ETHER	143	62	3.82	3.47 A	C18H20O5	2-HYOROXYNAPHTHOQUINONE,3-(W-ME-W-CARBOMETHOXYPENT)
5166	OOOECANE	475		5.07		C18H21CL1N2S1	BUTYL "CHLORPROMAZINE"
5167	OIETHYL ETHER	492	17	0.19	1.01 B	C18H21N1O3	COOEINE
5168	OIETHYL ETHER	3	17	-0.10	0.78 B	C18H21N1O3	COOEINE
5169	OIETHYL ETHER	359		0.03	0.88 B	C18H21N1O3	COOEINE
5170	CHCL3	493		1.94	1.42 B	C18H21N1O3	COOEINE
5171	CHCL3	359		2.17	1.63 B	C18H21N1O3	COOEINE
5172	1-BUTANOL	4		1.21	1.19	C18H21N1O3	COOEINE
5173	CCL4	492		-0.62		C18H21N1O3	COOEINE
5174	CLCH2CH2CL	492		-1.32		C18H21N1O3	COOEINE
5175	ETHYL OLEATE	494		1.29		C18H21N1O3	DICODIOE /OIHYOROCODIENONE/
5176	ETHYL OLEATE	494		1.37		C18H21N1O4	EUCOOAL /OXYCOOONE/
5177	CYCLOHEXANE	495		0.78		C18H21N3	BENZIMIDAZOLE,1-OIMETHYLAMINOETHYL,2-BENZYL
5178	OCTANOL	56		-0.15	-0.15 =	C18H22CL1N2S1	N-METHYLCHLORPROMAZINE CHLORIOE
5179	OCTANOL	483	44	4.28	4.28 =	C18H22N2	OESIPRAMINE
5180	OIETHYL ETHER	466		2.88	2.65 A	C18H22N2	OESIPRAMINE
5181	CHCL3	466		3.82	3.05 B	C18H22N2	OESIPRAMINE
5182	HEXANE	466		2.27		C18H22N2	OESIPRAMINE
5183	CHCL3	466		2.43	1.84 B	C18H22N2O1	10-HYOROXYOESIMIPRAMINE
5184	OIETHYL ETHER	466		2.00	1.87 A	C18H22N2O1	2-HYOROXYDESIPRAMINE
5185	CHCL3	466		1.99	1.48 B	C18H22N2O1	2-HYOROXYOESIPRAMINE
5186	HEXANE	466		0.72		C18H22N2O1	2-HYOROXYOESIPRAMINE
5187	OCTANOL	483	44	4.90	4.90 =	C18H22N2O1S1	METHOPROMAZINE
5188	N-HEPTANE	485	14	1.51		C18H22N2O1S1	METHOPROMAZINE
5189	CHCL3	482	68	0.71	1.27 N	C18H22N2O1S1	METHOXYPROMAZINE
5190	CHCL3	482	69	1.38	1.90 N	C18H22N2O1S1	METHOXYPROMAZINE
5191	OCTANOL	56		3.50	3.50 =	C18H22N2O2S2	PHENOTHIAZINE,2-MESULFONYL-10-(3-OIMEAMINOPROPYL)
5192	OCTANOL	127		2.65	2.65 =	C18H22N2O5S1	PENICILLIN,1-PHENOXYPROPYL/PROPICILLIN/
5193	OCTANOL	127		2.76	2.76 =	C18H22N2O5S1	PENICILLIN,2-PHENOXY-2-PROPYL
5194	1-BUTANOL	130	12	0.66	0.42	C18H22N2O5S1	PENICILLIN,1-PHENOXYPROPYL/PROPICILLIN/
5195	CHCL3	482	68	1.06	1.60 N	C18H22N2S1	TRIMEPRAZINE
5196	CHCL3	482	68	1.14	1.67 N	C18H22N2S2	THIOMETHYLPROMAZINE
5197	CHCL3	482	69	1.88	2.36 N	C18H22N2S2	THIOMETHYLPROMAZINE
5198	CYCLOHEXANE	141		3.45		C18H22O2S2	1,4-NAPHTHOQUINONE,2,3-OIBUTYLTHIO
5199	DIETHYL ETHER	496		-0.18	-0.04 A	C18H22O4	6-OXOESTRIOL
5200	ETHYL ACETATE	496		0.75	0.75	C18H22O4	6-OXOESTRIOL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5201	CHCL3	486	46	0.97	1.46 N	C18H23CL1N2O1S1	METHOXYPROMAZINE HYDROCHLORIDE
5202	N-HEPTANE	477		1.49		C18H23N1O1	ORPHENADRINE
5203	CYCLOHEXANE	141		3.44		C18H23N1O2S1	1,4-NAPHTHOQUINONE,2-BUTYLAMINO,3-BUTYLTHIO
5204	OLEYL ALCOHOL	142		2.57	3.14	C18H23N1O3	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N,N-DIALLYL
5205	DIETHYL ETHER	496		0.89	0.90 A	C18H24O3	ESTRIOL
5206	ETHYL ACETATE	496		1.38	1.43	C18H24O3	ESTRIOL
5207	DIETHYL ETHER	496		-0.92	-0.69 A	C18H24O4	6-A-HYDROXYESTRIOL
5208	ETHYL ACETATE	496		-0.05	-0.09	C18H24O4	6-A-HYDROXYESTRIOL
5209	CYCLOHEXANE	304		3.62		C18H24O5	DIETHYLMALONATE,3-BUTOXYBENZAL
5210	CHCL3	497		3.67	2.91 B	C18H25N1O1	DEXTROMETHORPHAN
5211	OLEYL ALCOHOL	489	27	2.56	3.10	C18H25N3O2	CINCHONINAMIDE,N-(2-DIETHYL-AMINOETHYL)-2-ETHOXY
5212	CHCL3	497	46	2.55		C18H26BR1N1O1	DEXTROMETHORPHAN HYDROBROMIDE
5213	CHCL3	497	46	1.77		C18H26CL1N1O1	DEXTROMETHORPHAN HYDROCHLORIDE
5214	CHCL3	497	46	3.11		C18H26I1N1O1	DEXTROMETHORPHAN HYDROIODIDE
5215	N-HEPTANE	498		-0.07		C18H26O2	TESTOSTERONE,19-NOR/NANDROLONE/
5216	CYCLOHEXANE	446	26	3.17		C18H27N1O1	N-NONYLCINNAMAMIDE
5217	N-HEPTANE	477		2.33		C18H27N1O2	CARAMIPHEN
5218	OLEYL ALCOHOL	142		3.07	3.61	C18H27N1O3	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N,N-DIPROPYL
5219	OLEYL ALCOHOL	142		1.42	1.97	C18H27N1O4	2-METHOXY-4-ALLYLPHENOXYETHOXYACETAMIDE,N,N-DIETHYL
5220	OLEYL ALCOHOL	142		1.26	1.81	C18H27N1O5	B-(2-MEO-4-ALLYLPHENOXY)-ETHANOLOXYACETAMIDE,N,N-DIET
5221	CHCL3	490	17	0.75	0.41 B	C18H28N2O1.HBR	1-(M-MEOBENZYL)-3-(N-DIETCARBAMOYL)PIPERIDINE
5222	CHCL3	490	17	0.51	0.20 B	C18H28N2O1.HBR	1-(P-MEOBENZYL)-3-(N-DIETCARBAMOYL)PIPERIDINE
5223	CHCL3	490	17	0.33	0.05 B	C18H28N2O2.HBR	1-(M-MEOBENZYL)-3-(N-DIETCARBAMOYL)PIPERIDINE
5224	CHCL3	490	17	0.30	0.03 B	C18H28N2O2.HBR	1-(P-MEOBENZYL)-3-(N-DIETCARBAMOYL)PIPERIDINE
5225	1-OCTANOL	353		-0.35		C18H29K1O3S1	POTASSIUM DODECYL BENZENESULFONATE
5226	1-OCTANOL	353		-0.45		C18H29NA1O3S1	SODIUM DODECYL BENZENESULFONATE
5227	OCTANE	57		3.74		C18H30O3	P-T-OCTYLPHENOXYMONOETHOXYETHANOL/OPE-1/
5228	CHCL3	464	46	2.97		C18H31N1O6S1	N-ME-3-ETHOXYCARBONYLPYRIDINIUM NONYLSULFATE
5229	CHCL3	464	46	3.06		C18H31N1O6S1	N-ME-3-METHOXYCARBONYLPYRIDINIUM DECYLSULFATE
5230	N-HEPTANE	479	31	5.08		C18H32O2	LINOLEIC ACID
5231	N-HEPTANE	479	31	5.36		C18H34O2	OLEIC ACID
5232	BENZENE	478		-0.42	0.26 B	C18H36N2O1	PIPERIDINE,1-DECYL,3-(N-ETHYLCARBAMYL)
5233	BENZENE	478		-0.70	0.06 B	C18H36N2O1	PIPERIDINE,1-DECYL,3-(N,N-DIMETHYLCARBAMYL(
5234	N-HEPTANE	479	31	5.43		C18H36O2	OCTADECANOIC ACID/STEARIC ACID/
5235	CHCL3	96		0.00		C19H15N1S2	TRIPHENYLSULFONIUM THIOCYANTE
5236	PARAFFINS	499		1.98		C19H16N2	N-PHENYL-P-PHENYLBENZAMIDINE
5237	PARAFFINS	499		2.16		C19H16N2	N-PHENYL-P-PHENYLBENZAMIDINE
5238	DIETHYL ETHER	143	62	4.43	4.00 A	C19H16O3	2-HYDROXYNAPHTHOQUINONE,3-(W-PHENYLPROPYL)
5239	1-BUTANOL	130		1.06	0.98	C19H17CL2N3O5S1	DICLOXACILLIN
5240	1-BUTANOL	130		0.75	0.55	C19H18CL1N3O5S1	CLOXACILLIN
5241	1-BUTANOL	130		0.59	0.32	C19H19N3O5S1	OXACILLIN
5242	OCTANOL	56		3.28	3.28 =	C19H20N2O3	OXYPHENBUTAZONE
5243	DIETHYL ETHER	143	62	5.45	4.90 A	C19H20O3	2-HYDROXYNAPHTHOQUINONE,3-(W-CYCLOHEXEN-3YL-PROPYL)
5244	HEXANE	456		0.99		C19H21CL1O6	7-CL-4,6-DIMEO-6'-ME-2'-PROPOXYGRIS-2'-EN-3,4'-DIONE
5245	HEXANE	456		1.38		C19H21CL1O6	7-CL-4,6-DIMEO-6'-ME-4'-PROPOXYGRIS-3'-EN-3,2'DIONE
5246	HEXANE	456		0.98		C19H21CL1O6	7-CL-6,2'-DIETO-4-MEO-6'-MEGRIS-2'-EN-3,4'-DIONE
5247	CHCL3	482	68	1.51	2.02 N	C19H21F3N2S1	RHODIA#7746/TRIFLUOTRIMEPRAZINE/
5248	CHCL3	482	69	2.02	2.49 N	C19H21F3N2S1	RHODIA#7746/TRIFLUOTRIMEPRAZINE/
5249	1-BUTANOL	4		2.02	2.34	C19H21N1O3	THEBAINE
5250	DIETHYL ETHER	3	17	1.21	1.91 B	C19H21N1O3	THEBAINE (PARAMORPHINE)
5251	OCTANOL	483	44	3.96	3.96 =	C19H21N1S1	DOSULEPINE
5252	CHCL3	482	68	0.64	1.21 N	C19H21N3S1	CYAMEPROMAZINE
5253	CHCL3	482	69	1.11	1.64 N	C19H21N3S1	CYAMEPROMAZINE
5254	OCTANOL	276		3.92	3.92 =	C19H22N2	TRIPROLIDINE /PKA = 9.50/
5255	CHCL3	482	68	0.59	1.16 N	C19H22N2O1S1	ACEPROMAZINE
5256	CHCL3	482	69	2.29	2.74 N	C19H22N2O1S1	ACEPROMAZINE
5257	N-HEPTANE	485	14	0.88		C19H22N2O1S1	ACEPROMAZINE
5258	N-HEPTANE	416	14	1.95		C19H22N2O6	BIS(P-AMINOSALICYLIC ACID) AMYL ESTER
5259	CHCL3	482	68	0.85	1.40 N	C19H22N2S1	MEPAZINE
5260	CHCL3	482	69	1.60	2.10 N	C19H22N2S1	MEPAZINE
5261	CHCL3	500	14	1.57		C19H22N4O3S1	THIAMINE,S-BENZOYL
5262	CHCL3	500	14	0.45		C19H22N4O3S2	THIAMINE,O-BENZOYL
5263	DIETHYL ETHER	143	62	5.93	5.31 A	C19H22O3	2-HYDROXYNAPHTHOQUINONE,3-(W-CYCLOHEXYLPROPYL)
5264	DIETHYL ETHER	465	62	3.92	3.56 A	C19H22O4	2-HYDROXYNAPHTHOQUINONE,3-(2-METHYLOCTYL-7-ONE)
5265	DIETHYL ETHER	465	62	3.20	2.93 A	C19H22O5	2-HYDROXYNAPHTHOQUINONE,3-(8-CARBOXYOCTYL)
5266	DIETHYL ETHER	465	62	4.10	3.72 A	C19H22O5	2-HYDROXYNAPHTHOQUINONE,3-(2-ME-6-CARBOMETHOXYHEX)
5267	OCTANOL	483	44	3.88	3.88 =	C19H23CL1N2	CHLORIMIPRAMINE
5268	DIETHYL ETHER	501	17	-0.88	0.07 B	C19H23N3O2	ERGOMETRINE/ERGONIVINE/
5269	DIETHYL ETHER	501	17	0.41	1.21 B	C19H23N3O2	ERGOMETRININE
5270	CHCL3	500	14	-2.40		C19H23N4O6P1S1	THIAMINE MONOPHOSPHATE,S-BENZOYL
5271	50%ETHER+50%DMF	125		0.23	1.37	C19H24CL1N1O1	2(A-ME-A-P-CLPHENYLBENZYL-OXY)-N,N-DIMEPROPYLAMINE
5272	OCTANOL	483	44	4.62	4.62 =	C19H24N2	IMIPRAMINE
5273	DIETHYL ETHER	466		2.75	2.54 A	C19H24N2	IMIPRAMINE
5274	CHCL3	466		3.30	2.60 B	C19H24N2	IMIPRAMINE
5275	HEXANE	466		2.82		C19H24N2	IMIPRAMINE
5276	CHCL3	466		1.69	1.22 B	C19H24N2O1	10-HYDROXYIMIPRAMINE
5277	DIETHYL ETHER	466		1.33	1.30 A	C19H24N2O1	2-HYDROXYIMIPRAMINE
5278	CHCL3	466		2.17	1.63 B	C19H24N2O1	2-HYDROXYIMIPRAMINE
5279	HEXANE	466		0.13		C19H24N2O1	2-HYDROXYIMIPRAMINE
5280	DIETHYL ETHER	466		-1.12	-0.86 A	C19H24N2O1	IMIPRAMINE-N-OXIDE
5281	CHCL3	466		1.54	1.10 B	C19H24N2O1	IMIPRAMINE-N-OXIDE
5282	HEXANE	466		-0.95		C19H24N2O1	IMIPRAMINE-N-OXIDE
5283	CHCL3	482	68	1.02	1.57 N	C19H24N2O1S1	METHOTRIMEPRAZINE
5284	CHCL3	482	69	1.93	2.41 N	C19H24N2O1S1	METHOTRIMEPRAZINE
5285	DIETHYL ETHER	378	44	0.99	1.80 B	C19H24N2O2	N,N-DIPHENYLCARBAMIC ACID,DIETAMINOETHYL ESTER
5286	DIETHYL ETHER	457	62	3.08	2.82 A	C19H24N2O2	1,4-NAPHTHOQUINONE,2-W-CYCLOHEXYLPROPYLHYDRAZINO
5287	CHCL3	482	68	1.29	1.81 N	C19H24N2S2	METHIOMEPRAZINE
5288	CHCL3	482	69	1.66	2.15 N	C19H24N2S2	METHIOMEPRAZINE
5289	CYCLOHEXANE	474	14	0.63		C19H24N4O2S2	THIAMINE BENZYL DISULFIDE
5290	CHCL3	474	14	1.42	1.00 B	C19H24N4O2S2	THIAMINE BENZYL DISULFIDE
5291	BENZENE	474	14	-1.52		C19H24N4O2S2	THIAMINE BENZYL DISULFIDE
5292	ETHYL ACETATE	474	14	1.68	1.77	C19H24N4O2S2	THIAMINE BENZYL DISULFIDE
5293	N-HEPTANE	498		0.34		C19H24O2	1,4-ANDROSTADIENE-3,17-DIONE
5294	N-HEPTANE	498		0.89		C19H24O2	4,6-ANDROSTADIENE-3,17-DIONE
5295	DIETHYL ETHER	143	62	6.70	5.98 A	C19H24O3	2-HYDROXYNAPHTHOQUINONE,3-NONYL
5296	DIETHYL ETHER	465	62	3.38	3.09 A	C19H24O4	2-HYDROXYNAPHTHOQUINONE,3-(7-OH-7-METHYLOCTYL)
5297	CHCL3	486	46	1.04	1.54 N	C19H25CL1N2O1S1	METHOTRIMEPRAZINE HYDROCHLORIDE
5298	CYCLOHEXANE	446		3.50		C19H25N1O1	N,N-DICYCLOPENTYLCINNAMAMIDE
5299	OCTANOL	235		3.83	3.83 =	C19H25N1O1	PROPOXYPHENE CARBINOL
5300	N-HEPTANE	421	44	3.64		C19H25N1O1	PROPOXYPHENE CARBINOL

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5301	CHCL3	482	68	-1.15	-0.47 N	C19H25N3S1	AMINOPPOMAZINE
5302	CHCL3	482	69	1.95	2.43 N	C19H25N3S1	AMINOPROMAZINE
5303	DIETHYL ETHER	457	62	3.93	3.57 A	C19H26N2O2	1,4-NAPHTHOQUINONE,2-NONYLHYDRAZINO
5304	N-HEPTANE	498		0.37		C19H26O2	4-ANDROSTENE-3,17-DIONE
5305	CHCL3	491	46	-2.00		C19H27BR1N1O3	ATROPINE-ETHYLBROMIDE
5306	OLEYL ALCOHOL	489	27	3.24	3.77	C19H27N3O2	CINCHONINAMIDE,N-(2-DIETHYL-AMINOETHYL)-2-PROPOXY
5307	CHCL3	464	46	2.98		C19H28BR1N1O4S1	N-METHYL-6-BROMOQUINOLINIUM NONYLSULFATE
5308	CHCL3	464	46	2.86		C19H28CL1N1O4S1	N-METHYL-6-CHLOROQUINOLINIUM NONYLSULFATE
5309	CHCL3	464	46	3.29		C19H28I1N1O4S1	N-METHYL-2-IODOQUINOLINIUM NONYLSULFATE
5310	N-HEPTANE	498		0.49		C19H28O2	EPITESTOSTERONE
5311	OCTANOL	261		3.32	3.32 =	C19H28O2	TESTOSTERONE
5312	OCTANOL	65		3.31	3.31 =	C19H28O2	TESTOSTERONE
5313	DIETHYL ETHER	502		1.94	3.20 S	C19H28O2	TESTOSTERONE
5314	N-HEPTANE	498		0.32		C19H28O2	TESTOSTERONE
5315	N-HEPTANE	477		2.51		C19H29N1C1	CYCRIMINE
5316	N-HEPTANE	477		1.75		C19H29N1O1	PROCYCLIDINE
5317	N-HEPTANE	498		-0.05		C19H29N1O2	TESTOSTERONE OXIME
5318	CHCL3	503	46	2.77		C19H29N1O4S1	N-METHYL-1-QUINOLINIUM NONYLSULFATE
5319	CHCL3	464	46	2.79		C19H29N1O4S1	N-METHYLQUINOLINIUM NONYLSULFATE
5320	CHCL3	464	46	3.13		C19H29N1O5S1	N-ME-8-OH-QUINOLINIUM NONYLSULFATE
5321	CHCL3	503	46	3.00		C19H30N2O4S1	1-METHYL-3-AMINOQUINOLINIUM NONYLSULFATE
5322	OLEYL ALCOHOL	473		4.28	4.85	C19H31N1O4	3-ETO-4-BUTOXYBENZOIC ACID,DIETHYLAMINOETHYL ESTER
5323	OLEYL ALCOHOL	473		3.78	4.35	C19H31N1O5	3,4,5-TRIETHOXYBENZOIC ACID,DIETHYLAMINOETHYL ESTER
5324	CHCL3	464	46	3.27		C19H33N1O6S1	N-ME-3-ETHOXYCARBONYLPYRIDINIUM DECYLSULFATE
5325	CHCL3	464	46	3.36		C19H33N1O6S1	N-ME-3-METHOXYCARBONYLPYRIDINIUM UNDECYLSULFATE
5326	OCTANOL	65	46	-0.08	-0.08 =	C19H34BR1N1	BENZYLDIMETHYLDECYLAMMONIUM BROMIDE
5327	OCTANOL	65	46	1.32	1.32 =	C19H34BR1N1	TETRADECYLPYRIDINIUM BROMIDE
5328	N-HEPTANE	443		3.30		C20H13N1S1	PHENOTHIAZINE,3,4,6,7-DIBENZO
5329	N-HEPTANE	443		5.26		C20H13N1S1	PHENOTHIAZINE,1,2,8,9-DIBENZO
5330	CHCL3	412		4.45		C20H16CU1N2O2	8-QUINOLINOLO(2-METHYL)(BIS)-CU(II)
5331	CHCL3	412		4.56		C20H16CU1N2O2	8-QUINOLINOLO(4-METHYL)(BIS)-CU(II)
5332	CCL4	412		3.29		C20H16CU1N2O2	8-QUINOLINOLO,4-METHYL(BIS)-CU(II)
5333	CCL4	412		3.50		C20H16CU1N2O2	8-QUINOLINOLO,2-METHYL(BIS)-CU(II)
5334	OCTANOL	227		1.74	1.74 =	C20H16N2O4	CAMPTOTHECIN (NCS 94600)
5335	DIETHYL ETHER	465	62	2.90	2.67 A	C20H16O4	2-HYDROXYNAPHTHOQUINONE,3-(3-P-TOLYLPROPYL-3-ONE)
5336	CYCLOHEXANE	141		4.40		C20H19N1O2S1	1,4-NAPHTHOQUINONE,2-ANILINO,3-BUTYLTHIO
5337	OCTANOL	227		3.67	3.67 =	C20H19N1O3	ACRONYCINE (NCS 403169)(PKA IN 40% MEOH= 3.40)
5338	1-BUTANOL	4		-1.15	-2.12	C20H19N1O5	BERBERINE
5339	OCTANOL	504	40	1.16	1.16 =	C20H19N1O8	4-DED(METHYLAMINOTETRACYCLINE
5340	OCTANOL	227	61	-1.85	-1.85 =	C20H22N8O5	METHOTREXATE (PKA IN 30% MEOH = 4.70)
5341	CHCL3	482	68	2.17	2.63 N	C20H23CL1N2S1	SANDOZ#6524
5342	HEXANE	456		1.27		C20H23CL1O6	2'-BUTOXY-7-CL-4,6-DIMEO-6'-MEGRIS-2'-EN-3,4'-DIONE
5343	HEXANE	456		1.72		C20H23CL1O6	4'-BUTOXY-7-CL-4,6-DIMEO-6'-MEGRIS-3'-EN-3,2'DIONE
5344	OCTANOL	483	44	4.92	4.92 =	C20H23N1	AMITRIPTYLINE
5345	CYCLOHEXANE	141		4.22		C20H23N1O4	A-CARBETHOXY-B-ANILINO-B-PHENYLPROPIONIC ACID,ET.EST.
5346	OILS	505	23	3.40		C20H24CL1N3O1	ACRIDINE,2-CL-7-MEO-5(2-DIETAMINO-2-ETAMINO)
5347	CHCL3	482	68	-0.70	-0.05 N	C20H24CL1N3S1	PROCHLORPERAZINE
5348	CHCL3	486		1.86	2.28 N	C20H24CL2N2S1	2-CL-10-(2(2-N-MEPIPERIDYL)ETHYL)PHENOTHIAZINE HCL
5349	CHCL3	482	68	1.44	1.95 N	C20H24N2O1S1	PROPIOMAZINE
5350	OCTANOL	186		1.73	1.73 =	C20H24N2O2	QUININE
5351	OCTANOL	218		1.83	1.83 =	C20H24N2O2	QUININE
5352	DIETHYL ETHER	3	17	1.64	1.65 A	C20H24N2O2	QUININE
5353	BENZENE	405	31	1.20	1.38 B	C20H24N2O2	QUININE
5354	DI-I-PR. ETHER	488		-1.60		C20H24N2O2	QUININE
5355	N-HEPTANE	416	14	1.98		C20H24N2O6	BIS(P-AMINOSALICYLIC ACID) HEXYL ESTER
5356	CHCL3	482	68	1.67	2.17 N	C20H24N2S1	SANDOZ#6457
5357	CYCLOHEXANE	495		1.86		C20H24N4O2	BENZIMIDAZOLE,1-DIETHYLAMINOETHYL,5-NITRO,2-BENZYL
5358	CYCLOHEXANE	495		2.06		C20H24N4O2	BENZIMIDAZOLE,1-DIETHYLAMINOETHYL,6-NITRO,2-BENZYL
5359	DIETHYL ETHER	143	62	4.97	4.49 A	C20H24O3	2-HYDROXYNAPHTHOQUINONE,3-(W-CARBOMETHOXYOCTYL)
5360	DIETHYL ETHER	143	62	6.70	5.98 A	C20H24O3	2-HYDROXYNAPHTHOQUINONE,3-(W-CYCLOHEXYLBUTYL)
5361	DIETHYL ETHER	465	62	4.27	3.87 A	C20H24O4	2-HYDROXYNAPHTHOQUINONE,3-(DECYL-7-ONE)
5362	CHCL3	486	46	-0.40	0.23 N	C20H25CL2N3S1	PROCHLORPERAZINE HYDROCHLORIDE
5363	OILS	505	23	2.61		C20H25N3	ACRIDINE,5-(DIETHYLAMINOPROPYLAMINO)
5364	CHCL3	482	68	-1.22	-0.53 N	C20H25N3S1	PERAZINE
5365	DIETHYL ETHER	143	62	7.29	6.50 A	C20H26O3	2-HYDROXYNAPHTHOQUINONE,3-DECYL
5366	DIETHYL ETHER	143	62	7.13	6.36 A	C20H26O3	2-HYDROXYNAPHTHOQUINONE,3-1-DECYL
5367	DIETHYL ETHER	143	62	2.67	2.46 A	C20H26O5	2-HYDROXYNAPHTHOQUINONE,3-(9,10-DIHYDROXYDECYL)
5368	N-HEPTANE	477		-3.49		C20H28N2O3	OXYPHENCYCLAMINE
5369	CHCL3	491	46	-1.32		C20H29BR1N1O3	ATROPINE-N-PROPYLBROMIDE
5370	OLEYL ALCOHOL	142		1.45	2.00	C20H29N1O2	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N-ALLYL-N-MEBUTYL
5371	OLEYL ALCOHOL	142		1.80	2.35	C20H29N1O2	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N,N-DIBUTYL
5372	OCTANOL	218		4.40	4.40 =	C20H29N3O2	DIBUCAINE/PERCAINE/
5373	OCTANOL	216	34	4.18	4.18 =	C20H29N3O2	DIBUCAINE/PERCAINE/
5374	OILS	462		3.50	3.40 B	C20H29N3O2	DIBUCAINE/PERCAINE/
5375	OLEYL ALCOHOL	489	27	3.70	4.23	C20H29N3O2	DIBUCAINE/PERCAINE/
5376	OCTANOL	216	79	2.18	2.18 =	C20H29N3O2.C2H4O2	DIBUCAINE ACETATE
5377	OCTANOL	216	56	1.97	1.97 =	C20H29N3O2.C8H6O4	DIBUCAINE PHTHALATE
5378	CHCL3	464	46	3.48		C20H30BR1N1O4S1	N-METHYL-6-BROMOQUINOLINIUM DECYLSULFATE
5379	CHCL3	464	46	3.30		C20H30CL1N1O4S1	N-METHYL-6-CHLOROQUINOLINIUM DECYLSULFATE
5380	CHCL3	464	46	3.79		C20H30I1N1O4S1	N-METHYL-2-IODOQUINOLINIUM DECYLSULFATE
5381	N-HEPTANE	498		0.72		C20H30O2	TESTOSTERONE,17-A-METHYL
5382	N-HEPTANE	477		3.02		C20H31N1O1	TRIHEXYLPHENIDYL
5383	OLEYL ALCOHOL	142		2.09	2.64	C20H31N1O3	2-METHOXY-4-ALLYLPHENOXYACETAMIDE,N,N-DI-I-BUTYL
5384	CHCL3	464	46	2.98		C20H31N1O4S1	1,2-DIMETHYLQUINOLINIUM NONYLSULFATE
5385	CHCL3	464	46	3.05		C20H31N1O4S1	1,4-DIMETHYLQUINOLINIUM NONYLSULFATE
5386	CHCL3	464	46	3.13		C20H31N1O4S1	1,6-DIMETHYLQUINOLINIUM NONYLSULFATE
5387	CHCL3	503	46	3.39		C20H31N1O4S1	1,8-DIMETHYLQUINOLINIUM NONYLSULFATE
5388	CHCL3	503	46	3.29		C20H31N1O4S1	N-METHYL-1-QUINOLINIUM DECYLSULFATE
5389	CHCL3	464	46	3.24		C20H31N1O4S1	N-METHYLQUINOLINIUM DECYLSULFATE
5390	OCTANOL	503	46	3.95	3.95 =	C20H31N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM OCTYLSULFATE
5391	CHCL3	464	46	3.02		C20H31N1O5S1	N-ME-6-METHOXYQUINOLINIUM NONYLSULFATE
5392	CHCL3	464	46	3.56		C20H31N1O5S1	N-ME-8-OH-QUINOLINIUM DECYLSULFATE
5393	CHCL3	464	46	3.31		C20H31N1O5S1	N-ME-8-METHOXYQUINOLINIUM NONYLSULFATE
5394	CHCL3	503	46	3.43		C20H32N2O4S1	1-METHYL-3-AMINOQUINOLINIUM DECYLSULFATE
5395	SEC-BUTANOL	84	19	-1.51	-2.62	C20H32N6O12S2	GLUTATHIONE DISULPHIDE
5396	N-BUTANOL	159		0.32	-0.10	C20H32N8	4-ANDROSTENE-3,17-DIONE-19-DEMETHYL
5397	OCTANOL	438		2.73	2.73 =	C20H32O6	GLUCOPYRANOSIDE,3,5-DI(T-BUTYL)PHENYL (BETA)
5398	OCTANE	57		3.14		C20H34O3	P-T-OCTYLPHENOXYD(ETHOXYETHANOL/OPE-2/
5399	CHCL3	464	46	3.19		C20H35N1O6S1	N-ME-3-BUTOXYCARBONYLPYRIDINIUM NONYLSULFATE
5400	CHCL3	464	46	3.60		C20H35N1O6S1	N-ME-3-ETHOXYCARBONYLPYRIDINIUM UNDECYLSULFATE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5401	CHCL3	464	46	3.72		C20H35N1O6S1	N-ME-3-METHOXYCARBONYLPYRIDINIUM DODECYLSULFATE
5402	BENZENE	478		-0.31	0.33 B	C20H38N2O1	PIPERIDINE,1-DECYL,3-(N-PYROLIDINO-FORMYL)
5403	BENZENE	478		-0.72	0.05 B	C20H38N2O2	PIPERIDINE,1-DECYL,3-(N-MORPHOLINO-FORMYL)
5404	BENZENE	478		-0.77	0.01 B	C20H40N2O1	PIPERIDINE,1-DECYL,4-(N,N-DIETHYLCARBAMYL) 81
5405	BENZENE	478	8	0.20	0.69 B	C20H40N2O1	PIPERIDINE,1-DECYL,3-(N,N-DIETHYLCARBAMYL)
5406	CHCL3	455		8.60		C21H18N4S1	THIOCARBAZONE,DI-A-NAPTHYL
5407	DIETHYL ETHER	465	62	3.90	3.54 A	C21H18O4	2-HYDROXYNAPHTHOQUINONE,3-(5-PHENYLPENTYL-5-ONE)
5408	PARAFFINS	499		2.76		C21H20N2O1	P-ETHOXY-N-(4-DIPHENYL)-BENZAMIDINE
5409	PARAFFINS	499		2.15		C21H20N2O1	P-PHENYL-N-(P-ETHOXYPHENYL)-BENZAMIDINE
5410	PARAFFINS	499		2.98		C21H20N2O2	3,4-DIMETHOXY-N-(4-DIPHENYL)-BENZAMIDINE
5411	OCTANOL	276		5.06	5.06 =	C21H20O3S1	1-(2-1-PROPYLPHENYLTHIOME)-3-CARBOXY-8-NAPHTHOL
5412	OCTANOL	504	40	-0.60	-0.60 =	C21H21CL1N2O8	DEMETHYLCHLORTETRACYCLINE
5413	I-BUTANOL	130	12	-0.66	-1.43	C21H21CL1N2O8	DEMETHYLCHLORTETRACYCLINE
5414	OCTANOL	218		1.93	1.93 =	C21H22N2O2	STRYCHNINE
5415	DIETHYL ETHER	3	17	0.34	1.16 B	C21H22N2O2	STRYCHNINE
5416	CHCL3	506		1.78	1.28 B	C21H22N2O2	STRYCHNINE
5417	DI-I-PR. ETHER	488		-0.21		C21H22N2O2	STRYCHNINE
5418	OCTANOL	504	40	-0.08	-0.08 =	C21H22N2O7	6-DEMETHYL-6-DEOXYTETRACYCLINE
5419	CHCL3	482	68	2.20	2.66 N	C21H23F3N2S1	SANDOZ#10-068
5420	CHCL3	482	69	3.18	3.58 N	C21H23F3N2S1	SANDOZ#10-068
5421	OCTANOL	218		1.03	1.03 =	C21H23N1O2	COLCHICEINE
5422	ETHYL OLEATE	494		1.07		C21H23N1O5	HEROIN /DIACETYL MORPHINE/
5423	CHCL3	482	68	0.52	1.09 N	C21H23N3O1S1	PROPERICIAZINE
5424	CHCL3	482	69	3.49	3.86 N	C21H23N3O1S1	PROPERICIAZINE
5425	CHCL3	482	68	-0.43	0.20 N	C21H24F3N3S1	TRIFLUOPERAZINE
5426	DODECANE	475		4.11		C21H24F3N3S1	TRIFLUOPERAZINE
5427	OCTANOL	469		1.84	1.84 =	C21H24N2O4	QUINAZOLIN-2-ONE,1-METHYL-4-PHENYL-6-TRIETHOXY
5428	OCTANOL	475	46	1.69	1.69 =	C21H25CL1F3N3S1	TRIFLUOPERAZINE HYDROCHLORIDE
5429	CHCL3	486	46	-0.15	0.45 N	C21H25CL1F3N3S1	TRIFLUOPERAZINE HYDROCHLORIDE
5430	N-HEPTANE	477		0.38		C21H25N1O1	BENZTROPINE
5431	OILS	505	23	2.37		C21H26CL1N3O1	ACRIDINE,2-CL-7-MEO-5(2-DIETAMINO-3-PR-AMINO)
5432	CHCL3	482	68	-1.40	-0.70 N	C21H26CL1N3O1S1	PERPHENAZINE
5433	CHCL3	482	68	1.50	2.01 N	C21H26N2O1S1	SANDOZ#KS33
5434	CHCL3	482	68	0.50	1.07 N	C21H26N2O1S2	MESORIDAZINE
5435	CHCL3	482	69	2.57	3.00 N	C21H26N2O1S2	MESORIDAZINE
5436	N-HEPTANE	416	14	2.19		C21H26N2O6	BIS(P-AMINOSALICYLIC ACID) HEPTYL ESTER
5437	CHCL3	482	68	2.04	2.51 N	C21H26N2S2	THIORIDAZINE
5438	DIETHYL ETHER	143	62	7.14	6.38 A	C21H26O3	2-HYDROXYNAPHTHOQUINONE,3-(W-CYCLOHEXYLPENTYL)
5439	I-BUTANOL	130		2.00	2.30	C21H26O5	PREDNISONE
5440	OCTANOL	227		1.46	1.46 =	C21H26O5	PREDNISONE (NCS 10023E)
5441	CHCL3	486	46	2.30		C21H27CL1N2S2	THIORIDAZINE HYDROCHLORIDE
5442	DIETHYL ETHER	502		0.29	1.62 S	C21H27F1O5	6-A-FLUORO-PREDNISOLONE
5443	DIETHYL ETHER	502		-0.12	1.21 S	C21H27F1O6	TRIAMCINOLONE
5444	ETHYL OLEATE	494		1.53		C21H27N1O1	METHADONE
5445	CYCLOHEXANE	495		1.30		C21H27N3O1	BENZIMIDAZOLE,1(2-DIME-AMINO,2-ME)ET,2-P-ETO-BENZYL
5446	CHCL3	482	68	-0.25	0.37 N	C21H27N3S2	SANDOZ#7834
5447	CHCL3	482	69	2.43	2.87 N	C21H27N3S2	SANDOZ#7834
5448	CHCL3	322		-1.38	-0.69 N	C21H27N7O5	NOR-PUROMYCIN (TYROSINE DERIVATIVE)
5449	N-HEPTANE	136	44	1.09		C21H28N2O3	HIRSUTINE/PSEUDO CONFIG./
5450	N-HEPTANE	136	44	0.78		C21H28N2O3	ISOCORYNANTHEIDINE/EPIALLO CONFIG./
5451	PRIM. PENTANOLS	181	10	-0.71		C21H28N7O17P3	NADP
5452	HEXANOL	181	18	-0.70		C21H28N7O17P3	NADP
5453	DIETHYL ETHER	143	62	7.69	6.86 A	C21H28O3	2-HYDROXYNAPHTHOQUINONE,3-1-UNDECYL
5454	DIETHYL ETHER	143	62	4.36	3.94 A	C21H28O4	2-HYDROXYNAPHTHOQUINONE,3-(W-DIMETHYL-W-OH-OCTYL)
5455	HEXANE	507		-1.52		C21H28O4	4-PREGNENE-21-OL,3,11,20-TRIONE
5456	DIETHYL ETHER	502		0.05	1.37 S	C21H28O5	PREDNISOLONE
5457	DIETHYL ETHER	508		0.00	0.84 B	C21H28O5	PREDNISOLONE
5458	OCTANOL	227		1.42	1.42 =	C21H28O5	PREDNISOLONE (NCS 9120E)
5459	OCTANOL	218		1.47	1.47 =	C21H28O5	4-PREGNENE,17-A,21-DIOL,3,11,20-TRIONE/CORTISONE/
5460	DIETHYL ETHER	502		0.15	1.47 S	C21H28O5	4-PREGNENE,17-A,21-DIOL,3,11,20-TRIONE/CORTISONE/
5461	BENZENE	507		-0.04	1.33 A	C21H28O5	4-PREGNENE,17-A,21-DIOL,3,11,20-TRIONE/CORTISONE/
5462	I-BUTANOL	130	12	1.80	2.02	C21H28O5	4-PREGNENE,17-A,21-DIOL,3,11,20-TRIONE/CORTISONE/
5463	DIETHYL ETHER	502		0.37	1.68 S	C21H29F1O5	9-A-FLUORO-HYDROCORTISONE
5464	DIETHYL ETHER	508		0.36	1.15 B	C21H29F1O5	9-A-FLUOROHYDROCORTISONE
5465	N-HEPTANE	477		2.79		C21H29N1O1	DIMETHYLAMINOETHYL-2-T-BUTYLBENZHYDRYL ETHER
5466	OCTANOL	261		3.87	3.87 =	C21H30O2	PROGESTERONE
5467	DIETHYL ETHER	502		2.78	4.01 S	C21H30O2	PROGESTERONE
5468	I-BUTANOL	130	12	2.40	2.86	C21H30O2	PROGESTERONE
5469	DIETHYL ETHER	502		1.72	2.99 S	C21H30O3	DESOXYCORTICOSTERONE
5470	OCTANOL	261		2.88	2.88 =	C21H30O3	4-PREGNENE-21-OL,3,20-DIONE/DEOXYCORTICOSTERONE/
5471	N-HEPTANE	498		0.56		C21H30O3	4-PREGNENE-21-OL,3,20-DIONE/DEOXYCORTICOSTERONE/
5472	HEXANE	507		0.39		C21H30O3	4-PREGNENE-21-OL,3,20-DIONE/DEOXYCORTICOSTERONE/
5473	N-HEPTANE	498		-1.18		C21H30O3	PROGESTERONE,11-A-HYDROXY
5474	N-HEPTANE	498		0.18		C21H30O3	PROGESTERONE,17-A-HYDROXY
5475	N-HEPTANE	498		-0.54		C21H30O3	PROGESTERONE,11-B-HYDROXY
5476	OCTANOL	261		2.46	2.46 =	C21H30O4	11-DESOXY-17-HYDROXYCORTICOSTERONE
5477	DIETHYL ETHER	502		0.66	1.97 S	C21H30O4	4-PREGNENE-11-B,21-DIOL-3,20-DIONE/CORTICOSTERONE/
5478	BENZENE	507		1.00	2.37 A	C21H30O4	4-PREGNENE,11-B,21-DIOL,3,20-DIONE/CORTICOSTERONE/
5479	DIETHYL ETHER	502		0.21	1.53 S	C21H30O5	HYDROCORTISONE
5480	DIETHYL ETHER	508		0.11	0.96 B	C21H30O5	HYDROCORTISONE
5481	BENZENE	507		-0.49	0.89 A	C21H30O5	HYDROCORTISONE
5482	I-BUTANOL	130		1.74	1.93	C21H30O5	HYDROCORTISONE
5483	CHCL3	491	46	-1.54		C21H31BR1N1O3	ATROPINE-N-BUTYROBROMIDE
5484	CYCLOHEXANE	446		4.14		C21H31N1O1	N-CYCLODODECYLCINNAMAMIDE
5485	OCTANOL	509	31	4.32	4.32 =	C21H31N1O3	3(N,N-DIMEAMME-2-NORBORNANYL)4-BUOXYBENZOATE/ENDO/
5486	OCTANOL	509	31	4.35	4.35 =	C21H31N1O3	3(N,N-DIMEAMME-2-NORBORNANYL)4-BUOXYBENZOATE/EXO/
5487	OLEYL ALCOHOL	489	28	4.41	4.98	C21H31N3O2	CINCHONINAMIDE,N-(2-DIETHYL-AMINOETHYL)-2-PENTOXY
5488	CHCL3	464	46	3.99		C21H32BR1N1O4S1	N-METHYL-6-BR-QUINOLINIUM UNDECYLSULFATE
5489	CHCL3	464	46	3.78		C21H32CL1N1O4S1	N-METHYL-6-CL-QUINOLINIUM UNDECYLSULFATE
5490	CHCL3	464	46	4.21		C21H32I1N1O4S1	N-ME-2-IODOQUINOLINIUM UNDECYLSULFATE
5491	CYCLOHEXANE	446		3.45		C21H33N1O1	N-DODECYLCINNAMAMIDE
5492	CHCL3	464	46	3.49		C21H33N1O4S1	1,2-DIMETHYLQUINOLINIUM DECYLSULFATE
5493	CHCL3	464	46	3.49		C21H33N1O4S1	1,4-DIMETHYLQUINOLINIUM DECYLSULFATE
5494	CHCL3	464	46	3.62		C21H33N1O4S1	1,6-DIMETHYLQUINOLINIUM DECYLSULFATE
5495	CHCL3	503	46	3.84		C21H33N1O4S1	1,8-DIMETHYLQUINOLINIUM DECYLSULFATE
5496	CHCL3	503	46	3.72		C21H33N1O4S1	N-METHYL-I-QUINOLINIUM UNDECYLSULFATE
5497	CHCL3	464	46	3.78		C21H33N1O4S1	N-METHYLQUINOLINIUM UNDECYLSULFATE
5498	OCTANOL	503	46	4.50	4.50 =	C21H33N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM NONYLSULFATE
5499	CHCL3	464	46	3.79		C21H33N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM NONYLSULFATE
5500	CHCL3	464	46	3.56		C21H33N1O5S1	N-ME-6-METHOXYQUINOLINIUM DECYLSULFATE

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5501	CHCL3	464	46	3.82		C21H33N1O5S1	N-ME-8-METHOXYQUINOLINIUM DECYLSULFATE
5502	CHCL3	464	46	4.04		C21H33N1O5S1	N-ME-8-OH-QUINOLINIUM UNDECYLSULFATE
5503	CHCL3	503	46	3.89		C21H34N2O4S1	1-METHYL-3-AMINOQUINOLINIUM UNDECYLSULFATE
5504	N-BUTANOL	159		0.99	0.86	C21H34N8	4-ANDROSTENE-3,17-DIONE
5505	CHCL3	464	46	3.56		C21H37N1O6S1	N-ME-3-BUTOXYCARBONYLPYRIDINIUM DECYLSULFATE
5506	CHCL3	464	46	3.96		C21H37N1O6S1	N-ME-3-ETHOXYCARBONYLPYRIDINIUM DODECYLSULFATE
5507	OCTANOL	65	46	1.83	1.83 =	C21H38BR1N1	HEXADECYLPYRIDINIUM BROMIDE
5508	OCTANOL	65	46	1.71	1.71 =	C21H38CL1N1	HEXADECYLPYRIDINIUM CHLORIDE
5509	NITROBENZENE	63		0.55	1.34	C21H38CL1N1O1	HEXADECYLPYRIDONIUM CHLORIDE
5510	CHCL3	464	46	3.23		C21H38N2O5S1	N-ME-3-FORMAMIDOPYRIDINIUM TETRADECYLSULFATE
5511	CHCL3	464	46	3.95		C21H39N1O4S1	1,2-DIMETHYLPYRIDINIUM TETRADECYLSULFATE
5512	N-BUTANOL	510		0.04	-0.45	C21H39N7O12	STREPTOMYCIN (AS TRI-P-TOLUENESULFONATE)
5513	BENZENE	478		0.26	0.73 B	C21H40N2O1	PIPERIDINE,1-DECYL,3-(N-PIPERIDINO-FORMYL)
5514	OCTANOL	141		3.38	3.38 =	C22H15N1O4S1	1,4-NAPHTHOQUINONE,2-ANILINO-3-PHENYLSULFONYL
5515	CYCLOHEXANE	141		2.45		C22H15N1O4S1	1,4-NAPHTHOQUINONE,2-ANILINO,3-PHENYLSULFONYL
5516	CYCLOHEXANE	334		2.39		C22H18N2O2	MALON-DIANILIDE,BENZAL
5517	OCTANOL	226	48	2.06	2.06 =	C22H21N1O2S1	3-TRITYLTHIO-L-ALANINE/NSC-83265/
5518	OCTANOL	504	40	-0.04	-0.04 =	C22H22N2O8	METHACYCLINE
5519	OCTANOL	504	40	-0.39	-0.39 =	C22H23CL1N2O8	CHLORTETRACYCLINE
5520	I-BUTANOL	130	12	-0.43	-1.11	C22H23CL1N2O8	CHLORTETRACYCLINE
5521	OCTANOL	504	40	-0.02	-0.02 =	C22H24N2O8	DOXYCYCLINE
5522	OCTANOL	218	39	-1.47	-1.47 =	C22H24N2O8	TETRACYCLINE
5523	OCTANOL	504	40	-1.25	-1.25 =	C22H24N2O8	TETRACYCLINE
5524	I-BUTANOL	130		-1.02	-1.91	C22H24N2O8	TETRACYCLINE
5525	OCTANOL	504	40	-1.12	-1.12 =	C22H24N2O9	OXYTETRACYCLINE
5526	N-HEPTANE	477		-0.74		C22H25N1O3	TROPINE BENZILATE
5527	CHCL3	482	68	-1.30	-0.61 N	C22H26F3N3O1S1	FLUPHENAZINE
5528	CHCL3	482	69	2.30	2.75 N	C22H26F3N3O1S1	FLUPHENAZINE
5529	DIETHYL ETHER	143	62	7.42	6.63 A	C22H26O3	2-HYDROXYNAPHTHOQUINONE,3-TR-4-CYCLOHEXYLCYCLOHEXYL
5530	CHCL3	486	46	-1.00	-0.32 N	C22H27CL1F3N3O1S1	FLUPHENAZINE HYDROCHLORIDE
5531	HEXANE	456		2.81		C22H27CL1O6	7-CL-4'-HEXOXY-4,6-DIMEO-6'-MEGRIS-3'-EN-3,2'DIONE
5532	OILS	505	23	2.39		C22H28CL1N3O1	ACRIDINE,2-CL-7-MEO-5(2-DIETAMINO-4-BU-AMINO)
5533	DIETHYL ETHER	502		0.87	2.16 S	C22H28F2O5	6-A-FLUORO-DEXAMETHASONE
5534	N-HEPTANE	136	44	1.54		C22H28N2O3	CORYNANTHEIDINE/ALLO CONFIG./
5535	N-HEPTANE	136	44	1.20		C22H28N2O3	DIHYDROCORYNANTHEINE/NORMAL CONFIG./
5536	N-HEPTANE	416	14	2.26		C22H28N2O6	BIS(P-AMINOSALICYLIC ACID) OCTYL ESTER
5537	CHCL3	482	68	2.29	2.74 N	C22H28N2S2	SANDOZ#TT418
5538	CYCLOHEXANE	495		1.99		C22H28N4O3	BENZIMIDAZOLE,1-DIET-AMINOET-2-(P-ETO-BENZYL)-5-NO2
5539	DIETHYL ETHER	502		1.51	2.78 S	C22H29F1O4	6-A-METHYL-9-A-FLUORO-21-DESOXYPREDNISOLONE
5540	DIETHYL ETHER	502		0.68	1.98 S	C22H29F1O5	BETAMETHASONE
5541	DIETHYL ETHER	502		0.59	1.90 S	C22H29F1O5	DEXAMETHASONE
5542	DIETHYL ETHER	508		0.82	1.59 B	C22H29F1O5	DEXAMETHASONE
5543	DIETHYL ETHER	502		0.62	1.93 S	C22H29F1O5	6-A-METHYL-9-A-FLUORO-PREDNISOLONE
5544	OCTANOL	235	67	4.18	4.18 =	C22H29N1O2	PROPOXYPHENE
5545	N-HEPTANE	421	44	3.65		C22H29N1O2	PROPOXYPHENE
5546	BENZENE	511		-0.36		C22H29N1O7	RHODOMYCIN
5547	CHCL3	482	68	0.02	0.62 N	C22H29N3S2	THIETHYLPERAZINE
5548	CHCL3	482	69	2.07	2.54 N	C22H29N3S2	THIETHYLPERAZINE
5549	CHCL3	322		0.89	1.36 N	C22H29N7O5	PUROMYCIN
5550	DIETHYL ETHER	143	62	8.24	7.34 A	C22H30O3	2-HYDROXYNAPHTHOQUINONE,3-DODECYL
5551	DIETHYL ETHER	502		0.54	1.85 S	C22H30O5	6-A-METHYL-PREDNISOLONE
5552	DIETHYL ETHER	508		0.42	1.20 B	C22H30O5	METHYLPREDNISOLONE
5553	DIETHYL ETHER	502		2.44	3.68 S	C22H31F1O3	9-A-FL-11-B-OH-6-A-MF-4-PREGNENE-3,20-DIONE
5554	DIETHYL ETHER	502		1.71	2.98 S	C22H31F1O4	6-A-METHYL-9-A-FLUORO-DESOXYHYDROCORTISONE
5555	CHCL3	491	46	-1.45		C22H33BR1N1O3	ATROPINE-N-AMYLBROMIDE
5556	OLEYL ALCOHOL	489	28	5.13	5.70	C22H33N3O2	CINCHONINAMIDE,N-(2-DIETHYL-AMINOETHYL)-2-HEXOXY
5557	CHCL3	464	46	4.40		C22H34BR1N1O4S1	N-METHYL-6-BR-QUINOLINIUM DODECYLSULFATE
5558	CHCL3	464	46	4.26		C22H34CL1N1O4S1	N-METHYL-6-CL-QUINOLINIUM DODECYLSULFATE
5559	CHCL3	464	46	4.65		C22H34I1N1O4S1	N-ME-2-IODOQUINOLINIUM DODECYLSULFATE
5560	CHCL3	464	46	3.93		C22H35N1O4S1	1,2-DIMETHYLQUINOLINIUM UNDECYLSULFATE
5561	CHCL3	464	46	3.95		C22H35N1O4S1	1,4-DIMETHYLQUINOLINIUM UNDECYLSULFATE
5562	CHCL3	464	46	4.06		C22H35N1O4S1	1,6-DIMETHYLQUINOLINIUM UNDECYLSULFATE
5563	CHCL3	503	46	4.29		C22H35N1O4S1	1,8-DIMETHYLQUINOLINIUM UNDECYLSULFATE
5564	CHCL3	503	46	4.15		C22H35N1O4S1	N-METHYL-1-QUINOLINIUM DODECYLSULFATE
5565	CHCL3	464	46	4.20		C22H35N1O4S1	N-METHYLQUINOLINIUM DODECYLSULFATE
5566	OCTANOL	503	46	5.05	5.05 =	C22H35N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM DECYLSULFATE
5567	CHCL3	464	46	4.20		C22H35N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM DECYLSULFATE
5568	CHCL3	464	46	3.98		C22H35N1O5S1	N-ME-6-METHOXYQUINOLINIUM UNDECYLSULFATE
5569	CHCL3	464	46	4.29		C22H35N1O5S1	N-ME-8-METHOXYQUINOLINIUM UNDECYLSULFATE
5570	CHCL3	464	46	4.50		C22H35N1O5S1	N-ME-8-OH-QUINOLINIUM DODECYLSULFATE
5571	CHCL3	503	46	4.33		C22H36N2O4S1	1-METHYL-3-AMINOQUINOLINIUM DODECYLSULFATE
5572	OCTANE	57		2.50		C22H38O5	P-T-OCTYLPHENOXYTRIETHOXYETHANOL/OPE-3/
5573	CHCL3	464	46	3.91		C22H39N1O6S1	N-ME-3-BUTOXYCARBONYLPYRIDINIUM UNDECYLSULFATE
5574	CHCL3	464	46	4.30		C22H39N1O6S1	N-ME-3-METHOXYCARBONYLPYRIDINIUM TETRADECYLSULF
5575	CHCL3	464	46	4.46		C22H41N1O4S1	1,2,5-TRIMETHYLPYRIDINIUM TETRADECYLSULFATE
5576	BENZENE	478		0.26	0.73 B	C22H44N2O1	PIPERIDINE,1-DECYL,3-(N,N,-DIPROPYLCARBAMYL)
5577	CYCLOHEXANE	141		4.00		C23H18N2O2	1,4-NAPHTHOQUINONE,2-ANILINO,3-P-TOLUIDINO
5578	OCTANOL	56		2.30	2.30 =	C23H20N2O3S1	SULFINPYRAZONE
5579	DIETHYL ETHER	143	62	5.77	5.19 A	C23H22O3	2-HYDROXYNAPHTHOQUINONE,3-W-B-TETRALYLPROPYL
5580	OCTANOL	268		0.62	0.62 =	C23H25CL1N2	MALACHITE GREEN
5581	DIETHYL ETHER	3	17	-0.74	0.19 B	C23H26N2O4	BRUCINE
5582	N-BUTANOL	253	36	0.11	-0.36	C23H26N2O4	BRUCINE
5583	I-BUTANOL	4		1.32	1.35	C23H26N2O4	BRUCINE
5584	DIETHYL ETHER	502		2.39	3.63 S	C23H27CL1F2O6	6,9-A-DIFLUORO-16-A-CL-PREDNISOLONE ACETATE
5585	DIETHYL ETHER	502		1.93	3.19 S	C23H27F3O6	6,9,16-A-TRIFLUORO-PREDNISOLONE ACETATE
5586	OCTANOL	504	40	-0.04	-0.04 =	C23H27N3O7	9-DIMEAMINO-6-DEMETHYL-6-DEOXYTETRACYCLINE
5587	OCTANOL	504	40	0.05	0.05 =	C23H27N3O7	MINOCYCLINE
5588	DIETHYL ETHER	502		1.66	2.92 S	C23H28F2O6	6-A-16-A-DIFLUORO-PREDNISOLONE ACETATE
5589	DIETHYL ETHER	143	62	7.37	6.59 A	C23H28O3	2-HYDROXYNAPHTHOQUINONE,3-W-TR-B-DECALYLPROPYL
5590	CHCL3	486	46	0.67	1.20 N	C23H29CL2N3O2S1	THIOPROPAZATE HYDROCHLORIDE
5591	DIETHYL ETHER	502		1.57	2.86 S	C23H29F1O6	6-A-FLUORO-PREDNISOLONE ACETATE
5592	CHCL3	482	68	-1.40	-0.70 N	C23H29N3O2S1	ACETOPHENAZINE
5593	CHCL3	482	69	1.71	2.20 N	C23H29N3O2S1	ACETOPHENAZINE
5594	BENZENE	435	46	-0.64		C23H30BR1N1O3	PROPANTHELINE BROMIDE
5595	OILS	505	23	2.41		C23H30CL1N3O1	ACRIDINE,2-CL-7-MEO-5(2-DIETAMINO-5-AM-AMINO)
5596	DIETHYL ETHER	502		1.91	3.17 S	C23H30F2O5	6-A-9-A-DIFLUORO-21-DESOXY-HYDROCORTISONE ACETATE
5597	CHCL3	482	68	2.29	2.74 N	C23H30N2O1S1	SANDOZ#KS75
5598	N-HEPTANE	136	44	1.38		C23H30N2O4	MITRACILIATINE/PSUEDO CONFIG
5599	N-HEPTANE	136	44	2.02		C23H30N2O4	MITRAGYNINE/ALLO CONFIG./
5600	N-HEPTANE	136	44	0.95		C23H30N2O4	SPECIOCILIATINE/EPIALLO CONFIG./

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5601	N-HEPTANE	136	44	1.49		C23H30N2O4	SPECIOGYNINE/NORMAL CONFIG./
5602	N-HEPTANE	416	14	2.32		C23H30N2O6	BIS(P-AMINOSALICYLIC ACID) NONYL ESTER
5603	CHCL3	512	57	1.05		C23H30N3O7	XANTHOMYCIN
5604	DIETHYL ETHER	502		1.40	2.68 S	C23H30O6	CORTISONE ACETATE
5605	DIETHYL ETHER	502		1.33	2.61 S	C23H30O6	PREDNISOLONE ACETATE
5606	DIETHYL ETHER	508		1.11	1.85 B	C23H30O6	PREDNISOLONE ACETATE
5607	DIETHYL ETHER	502		1.66	2.92 S	C23H31F1O6	9-A-FLUORO-HYDROCORTISONE ACETATE
5608	DIETHYL ETHER	508		1.23	1.95 B	C23H31F1O6	9-A-FLUOROHYDROCORTISONE ACETATE
5609	OCTANOL	56		3.47	3.47 =	C23H31N1O2	A,A-DIPHENYLVALERIC ACID, DIETHYLAMINOETHYL ESTER
5610	OCTANOL	276		4.65	4.65 =	C23H31N1O2	SKF 525A /PKA = 8.80/
5611	CHCL3	464	46	4.65		C23H31N1O4S1	N-METHYLACRIDINIUM NONYLSULFATE
5612	CYCLOHEXANE	495		1.48		C23H31N3O1	BENZIMIDAZOLE,1(2-DIET-AMINO,2-ME)ET,2-P-ETO-BENZYL
5613	DIETHYL ETHER	502		1.42	2.70 S	C23H32O6	HYDROCORTISONE ACETATE
5614	DIETHYL ETHER	513		1.09	2.37 S	C23H32O6	HYDROCORTISONE ACETATE
5615	DIETHYL ETHER	508		1.11	1.85 B	C23H32O6	HYDROCORTISONE ACETATE
5616	I-BUTANOL	130		0.95	0.83	C23H32O6	G-STROPHANTHIDIN
5617	CHCL3	405	46	-0.70		C23H33I1N2O1	ISOPROPAMIDE
5618	N-BUTANOL	159		0.70	0.46	C23H34N8O3	PREDNISONEDIGUANYLHYDRAZONE
5619	I-BUTANOL	130		1.95	2.20	C23H34O4	DIGITOXIGENIN
5620	CHCL3	491	46	-0.74		C23H35BR1N1O3	ATROPINE-N-HEXYLBROMIDE
5621	N-BUTANOL	159		1.54	1.62	C23H36N8	D-1-PROGESTERONEDIGUANYLHYDRAZONE
5622	N-BUTANOL	159		1.47	1.52	C23H36N8	D-6-PROGESTERONEDIGUANYLHYDRAZONE
5623	N-BUTANOL	159		0.82	0.62	C23H36N8O1	D-6-PROGESTERONE-14-OH/DIGUANYLHYDRAZONE/
5624	N-BUTANOL	159		1.02	0.90	C23H36N8O1	PROGESTERONEDIGUANYLHYDRAZONE,11-ONE
5625	N-BUTANOL	159		1.58	1.68	C23H36N8O2	D-1,6-PROGESTERONEDIGUANYLHYDRAZONE
5626	N-BUTANOL	159		0.38	0.01	C23H36N8O3	CORTISONEDIGUANYLHYDRAZONE
5627	N-BUTANOL	159		0.51	0.19	C23H36N8O3	CORTISONEDIGUANYLHYDRAZONE
5628	N-BUTANOL	159		0.59	0.30	C23H36N8O3	PREDISOLONEDIGUANYLHYDRAZONE
5629	N-BUTANOL	159		0.99	0.86	C23H36N10O2	PROGESTERONEDIGUANYLHYDRAZONE,2,4-DI-NITROSO
5630	N-BUTANOL	159		1.65	1.71	C23H37CL1N8	4-CHLOROPROGESTERONE/DIGUANYLHYDRAZONE/
5631	CHCL3	464	46	4.35		C23H37N1O4S1	1,2-DIMETHYLQUINOLINIUM DODECYLSULFATE
5632	CHCL3	464	46	4.58		C23H37N1O4S1	1.6-DIMETHYLQUINOLINIUM DODECYLSULFATE
5633	CHCL3	503	46	4.73		C23H37N1O4S1	1,8-DIMETHYLQUINOLINIUM DODECYLSULFATE
5634	CHCL3	464	46	4.42		C23H37N1O4S1	1,4-DIMETHYLQUNIOLINIUM DODECYLSULFATE
5635	OCTANOL	503	46	5.45	5.45 =	C23H37N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM UNDECYLSULFATE
5636	CHCL3	464	46	4.66		C23H37N1O4S1	1,2,6-TRIMETHYLQUINOLINIUM UNDECYLSULFATE
5637	CHCL3	464	46	4.52		C23H37N1O5S1	N-ME-6-METHOXYQINOLINIUM DODECYLSULFATE
5638	CHCL3	464	46	4.77		C23H37N1O5S1	N-ME-8-METHOXYQINOLINIUM DODECYLSULFATE
5639	N-BUTANOL	159		1.52	1.59	C23H38N8	PROGESTERONEDIGUANYLHYDRAZONE
5640	N-BUTANOL	159		0.88	0.71	C23H38N8O1	PROGESTERONEDIGUANYLHYDRAZONE,11-OH
5641	N-BUTANOL	159		0.93	0.78	C23H38N8O1	PROGESTERONEDIGUANYLHYDRAZONE,17-OH
5642	N-BUTANOL	159		1.12	1.04	C23H38N8O1	PROGESTERONEDIGUANYLHYDRAZONE,21-OH
5643	N-BUTANOL	159		0.34	-0.04	C23H38N8O2	PROGESTERONEDIGUANYLHYDRAZONE,7,14-DI-OH
5644	N-BUTANOL	159		0.51	0.19	C23H38N8O2	PROGESTERONEDIGUANYLHYDRAZONE,6,11-DI-OH
5645	N-BUTANOL	159		0.54	0.24	C23H38N8O2	PROGESTERONEDIGUANYLHYDRAZONE,11,17-DI-OH
5646	N-BUTANOL	159		0.59	0.29	C23H38N8O2	PROGESTERONEDIGUANYLHYDRAZONE,16,17-DI-OH
5647	N-BUTANOL	159		0.75	0.53	C23H38N8O2	PROGESTERONEDIGUANYLHYDRAZONE,17,21-DI-OH
5648	N-BUTANOL	159		0.31	-0.08	C23H38N8O3	HYDROCORTISONEDIGUANYLHYDRAZONE
5649	N-BUTANOL	159		1.11	1.03	C23H40N8	3,20-PREGNANEDIONEDIGUANYLHYDRAZONE,5-H-CIS
5650	N-BUTANOL	159		1.06	0.96	C23H40N8	3,20-PREGNANEDIONEDIGUANYLHYDRAZONE,5-H-TRANS
5651	N-BUTANOL	159		0.76	0.52	C23H40N8O1	PREGNANE-3,20-DIONE-12-OH/DIGUANYLHYDRAZONE/
5652	CHCL3	464	46	4.27		C23H41N1O6S1	N-ME-3-BUTOXYCARBONYLPYRIDINIUM DODECYLSULFATE
5653	CHCL3	464	46	4.60		C23H41N1O6S1	N-ME-3-ETHOXYCARBONYLPYRIDINIUM TETRADECYLSULFA
5654	OCTANOL	65	46	2.72	2.72 =	C23H42BR1N1	OCTADECYLPYRIDINIUM BROMIDE
5655	N-BUTANOL	514		0.61	0.35	C23H46H6O13	NEOMYCIN-B (AS 2-ETHYL BUTYRATE)
5656	CHCL3	95	46	0.68		C24H20AS1BR1	TETRAPHENYLARSONIUM BROMIDE
5657	CHCL3	95	46	-0.74		C24H20AS1CL1	TETRAPHENYLARSONIUM CHLORIDE
5658	CHCL3	95	46	-0.74		C24H20AS1N1O2	TETRAPHENYLARSONIUM NITRITE
5659	CHCL3	95	46	1.88		C24H20AS1N1O3	TETRAPHENYLARSONIUM NITRATE
5660	CHCL3	97	46	0.50		C24H20BR1P1	TETRAPHENYLPHOSPHONIUM BROMIDE
5661	CHCL3	97	46	-0.33		C24H20BR1O3P1	TETRAPHENYLPHOSPHONIUM BROMATE
5662	CHCL3	97	46	-0.74		C24H20CL1P1	TETRAPHENYLPHOSPHONIUM CHLORIDE
5663	CHCL3	97	46	1.85		C24H20I1P1	TETRAPHENYLPHOSPHONIUM IODIDE
5664	CHCL3	97	46	-0.96		C24H20N1O2P1	TETRAPHENYLPHOSPHONIUM NITRITE
5665	CHCL3	97	46	0.67		C24H20N1O3P1	TETRAPHENYLPHOSPHONIUM NITRATE
5666	CHCL3	95	46	-1.30		C24H21AS1O3S1	TETRAPHENYLARSONIUM SULFITE
5667	CHCL3	95	46	-1.79		C24H21AS1O3S2	TETRAPHENYLARSONIUM THIOSULFATE
5668	CHCL3	95	46	-0.23		C24H22AS1CR1O4	TETRAPHENYLARSONIUM CHROMATE
5669	CHCL3	95	46	1.09		C24H22AS1CR1O4	TETRAPHENYLARSONIUM CHROMATE
5670	CHCL3	95	46	-2.00		C24H22AS1O4P1	TETRAPHENYLARSONIUM PHOSPHATE
5671	CHCL3	97	46	-0.29		C24H22CR1O4P1	TETRAPHENYLPHOSPHONIUM CHROMATE
5672	CHCL3	97	46	0.73		C24H22CR1O4P1	TETRAPHENYLPHOSPHONIUM CHROMATE
5673	CHCL3	97	46	-1.60		C24H22O4P2	TETRAPHENYLPHOSPHONIUM PHOSPHATE
5674	PARAFFINS	499		2.10		C24H25N3	P-PHENYL-N-(P-PIPERIDINOPHENYL)-BENZAMIDINE
5675	CHCL3	497	46	6.70		C24H28N4O8	DEXTROMETHORPHAN PICRATE
5676	CCL4	497	46	4.20		C24H28N4O8	DEXTROMETHORPHAN PICRATE
5677	DIETHYL ETHER	508		1.23	1.95 B	C24H30F2O6	FLUOCINOLONE ACETONIDE
5678	DIETHYL ETHER	502		2.16	3.40 S	C24H30F2O6	6-A-FLUORO-DEXAMETHASONE ACETATE
5679	DIETHYL ETHER	502		1.41	2.69 S	C24H30F2O6	6-A-FLUORO-TRIAMCINOLONE ACETONIDE
5680	DIETHYL ETHER	502		1.97	3.23 S	C24H31F1O5	6-A-METHYL-9-A-FLUORO-21-DEOXYPREDNISOLONE ACETATE
5681	DIETHYL ETHER	502		1.92	3.18 S	C24H31F1O6	6-A-METHYL-9-A-FLUORO-PREDNISOLONE ACETATE
5682	DIETHYL ETHER	502		1.16	2.44 S	C24H31F1O6	TRIAMCINOLONE ACETONIDE
5683	DIETHYL ETHER	513		1.11	2.39 S	C24H31F1O6	TRIAMCINOLONE ACETONIDE
5684	DIETHYL ETHER	508		1.10	1.84 B	C24H31F1O6	TRIAMCINOLONE ACETONIDE
5685	CHCL3	482	68	-0.11	0.50 N	C24H31N3O1S1	BUTAPERAZINE
5686	CHCL3	482	69	1.32	1.84 N	C24H31N3O1S1	BUTAPERAZINE
5687	CHCL3	482	68	-0.89	-0.22 N	C24H31N3O2S1	CARPHENAZINE
5688	CHCL3	482	69	1.89	2.37 N	C24H31N3O2S1	CARPHENAZINE
5689	OILS	505	23	2.29		C24H32CL1N3O1	ACRIDINE,2-CL-7-MEO-5(2-DIETAMINO-6-HEX-AMINO)
5690	N-HEPTANE	416	14	2.36		C24H32N2O6	BIS(P-AMINOSALICYLIC ACID) DECYL ESTER
5691	DIETHYL ETHER	502		1.83	3.09 S	C24H32O6	6-A-METHYL-PREDNISOLONE ACETATE
5692	DIETHYL ETHER	513		0.82	2.11 S	C24H32O6	PREDNACINOLONE
5693	DIETHYL ETHER	508		1.09	1.81 B	C24H33F1O6	FLUANDRENOLONE ACETONIDE
5694	CYCLOHEXANE	474	14	-2.30		C24H34N8O4S2	THIAMINE DISULFIDE
5695	CHCL3	474	14	-1.49	-1.50 B	C24H34N8O4S2	THIAMINE DISULFIDE
5696	ETHYL ACETATE	474	14	-1.03	-1.16	C24H34N8O4S2	THIAMINE DISULFIDE
5697	CHCL3	491	46	-0.30		C24H37BR1N1O3	ATROPINE N-HEPTYLBROMIDE
5698	N-BUTANOL	159		1.00	0.87	C24H37N8O2	PROGESTERONEDIGUANYLHYDRAZONE,16-CARBOXY
5699	N-BUTANOL	159		0.33	-0.05	C24H37N9	PROGESTERONEDIGUANYLHYDRAZONE,5-CYANO
5700	N-BUTANOL	159		0.61	0.33	C24H37N9	PROGESTERONEDIGUANYLHYDRAZONE,12-CYANO

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5701	OCTANOL	503	46	5.90	5.90 =	C24H39N104S1	1,2,6-TRIMETHYLQUINOLINIUM DODECYLSULFATE
5702	CHCL3	464	46	5.13		C24H39N104S1	1,2,6-TRIMETHYLQUINOLINIUM DODECYLSULFATE
5703	OCTANE	57		2.03		C24H42O6	P-T-OCTYLPHENOXYTETRAETHOXYETHANOL/OPE-4/
5704	CHCL3	95		1.53		C25H20AS1N1S1	TETRAPHENYLARSONIUM THIOCYANATE
5705	OCTANOL	268	59	0.96	0.96 =	C25H30CL1N3	GENTIAN VIOLET/CRYSTAL VIOLET/
5706	DIETHYL ETHER	502		1.54	2.81 S	C25H33F1O6	6-A-METHYL-TRIAMCINOLONE ACETONIDE
5707	OCTANOL	283	7	-1.37	-1.37 =	C25H33N1O4.HCL	ETORPHINE HYDROCHLORIDE
5708	OILS	505	23	2.18		C25H34CL1N3OI	ACRIDINE,2-CL-7-MEO-5(2-DIETAMINO-7-HEP-AMINO)
5709	DIETHYL ETHER	502		2.40	3.64 S	C25H34O5	6-A-METHYL-21-DESOXY-PREDNISOLONE PROPIONATE
5710	DIETHYL ETHER	502		1.73	3.00 S	C25H35F1O6	6-A-METHYL-9-A-FLUORO-16-A-HYDROXYCORTISONE ACETONIDE
5711	CHCL3	464	46	5.45		C25H35N1O4S1	N-METHYLACRIDINIUM UNDECYLSULFATE
5712	DIETHYL ETHER	502		2.39	3.63 S	C25H36O6	HYDROCORTISONE-21-BUTYRATE
5713	DIETHYL ETHER	502		2.35	3.59 S	C25H36O6	HYDROCORTISONE-21-I-BUTYRATE
5714	CHCL3	491	46	0.22		C25H39BR1N1O3	ATROPINE-N-OCTYLBROMIDE
5715	CHCL3	515	41	3.42		C25H41N1O7S1	HOMATROPINE-NONYLSULFATE
5716	CHCL3	464	46	5.12		C25H45N1O6S1	N-ME-3-BUTOXYCARBONYLPYRIDINIUM TETRADECYLSULF.
5717	OCTANOL	65	46	3.28	3.28 =	C25H46BR1N1	BENZYLDIMETHYLHEXADECYLAMMONIUM BROMIDE
5718	TOLUENE	148		0.04	0.68 B	C26H22CD1N8O2	CADMIUM-CARBAZONE COMPLEX
5719	TOLUENE	148		2.95	2.82 B	C26H22CU1N8O2	CUPRIC-CARBAZONE COMPLEX
5720	TOLUENE	148		3.08	2.86 B	C26H22FE1N8O2	FERROUS-CARBAZONE COMPLEX
5721	TOLUENE	148		-0.30	0.44 B	C26H22MN1N8O2	MANGANOUS-CARBAZONE COMPLEX
5722	TOLUENE	148		1.18	1.49 B	C26H22N8O2PB1	PLUMBOUS-CARBAZONE COMPLEX
5723	TOLUENE	148		2.30	2.33 B	C26H22N8O2SN1	STANNOUS-CARBAZONE COMPLEX
5724	TOLUENE	148		0.11	0.73 B	C26H22N8O2ZN1	ZINC-CARBAZONE COMPLEX
5725	TOLUENE	148		-0.10	0.58 B	C26H22NI1N8O2	NICKEL-CARBAZONE COMPLEX
5726	DIETHYL ETHER	502		3.18	4.39 S	C26H34F2O6	6-A-FLUORO-DEXAMETHASONE-21-BUTYRATE
5727	DIETHYL ETHER	502		3.24	4.45 S	C26H34F2O6	6-A-FLUORO-DEXAMETHASONE-21-I-BUTYRATE
5728	CHCL3	491	46	0.87		C26H41BR1N1O3	ATROPINE-N-NONYLBROMIDE
5729	OCTANE	57		1.61		C26H46O7	P-T-OCTYLPHENOXYPENTAETHOXYETHANOL/OPE-5/
5730	CHCL3	516	64	1.08		C27H28BR2O5S1	BROMTHYMOLBLUE
5731	BENZENE	516	64	0.45		C27H28BR2O5S1	BROMTHYMOLBLUE
5732	TOLUENE	516	64	0.30		C27H28BR2O5S1	BROMTHYMOLBLUE
5733	CCL4	516	64	0.10		C27H28BR2O5S1	BROMTHYMOLBLUE
5734	CLCH2CH2CL	516	64	0.91		C27H28BR2O5S1	BROMTHYMOLBLUE
5735	DIETHYL ETHER	502		2.93	4.15 S	C27H35F1O7	6-A-ME-9-A-FL-PREDNISOLONE-16,17-ACETONIDE-21-ACETATE
5736	DIETHYL ETHER	502		2.71	3.94 S	C27H37F1O6	BETAMETHASONE-17-VALERATE
5737	DIETHYL ETHER	513	12	0.11	1.43 S	C27H37F1O6	BETAMETHASONE-17-VALERATE
5738	DIETHYL ETHER	502		2.98	4.20 S	C27H37F1O7	6-A-ME-9-A-FL-HYDROXYCORTISONE-ACETONIDE-21-ACETATE
5739	DIETHYL ETHER	502		3.56	4.75 S	C27H40O6	HYDROCORTISONE-21-CAPROATE
5740	CHCL3	491	46	1.15		C27H43BR1N1O3	ATROPINE-N-DECYLBROMIDE
5741	DIETHYL ETHER	502		3.23	4.44 S	C28H37F1O7	6-A-METHYL-TRIAMCINOLONE ACETONIDE-21-PROPIONATE
5742	DIETHYL ETHER	502		3.14	4.35 S	C28H39F1O7	6-A-ME-9-A-FL-HYDROXYCORTISONE-ACETONIDE-PROPIONATE
5743	MIXED SOLV#1	433		2.78		C28H48N2O3	BARBITURIC ACID,1-N-OCTADECYL-5,5-DIALLYL
5744	OCTANE	57		1.23		C28H50O8	P-T-OCTYLPHENOXYHEXAETHOXYETHANOL/OPE-6/
5745	DIETHYL ETHER	517	19	0.80		C30H30N4O4	DEUTERO-PORPHYRIN
5746	HEXANE	456		-1.17		C30H33CL1O15	GRISEOFULVIN,TETRA-ACETYL-2'-GLUCOSYLOXY
5747	CHCL3	515	41	4.07		C30H45N1O7S1	METHANTHELINE-NONYLSULFATE
5748	CHCL3	515	41	4.66		C30H53N1O7S1	OXYPHENONIUM-NONYLSULFATE
5749	OCTANE	57		0.74		C30H54O9	P-T-OCTYLPHENOXYHEPTAETHOXYETHANOL/OPE-7/
5750	CHCL3	515	41	4.90		C30H55N1O5S1	TRIDIHEXYL-NONYLSULFATE
5751	OCTANOL	65	46	-1.47	-1.47 =	C31H32BR2N6O1	NCS-113089
5752	CYCLOHEXANE	141		3.27		C31H46O2	1,4-NAPHTHOQUINONE,2-METHYL,3-PHYTYL (VITAMIN K)
5753	CHCL3	515	41	3.95		C31H50N2O6S1	BENZOMETHAMINE-NONYLSULFATE
5754	CHCL3	515	41	5.60		C32H49N1O7S1	PROPANTHELINE-NONYLSULFATE
5755	DIETHYL ETHER	3	17	2.45	2.26 A	C32H49N1O9	CEVADINE
5756	I-BUTANOL	4		2.17	2.54	C32H49N1O9	CEVADINE
5757	CHCL3	515	41	4.49		C32H52N2O5S1	ISOPROPAMIDE-NONYLSULFATE
5758	OCTANE	57		0.30		C32H58O10	P-T-OCTYLPHENOXYOCTAETHOXYETHANOL/OPE-8/
5759	DIETHYL ETHER	517	19	1.23		C34H34N4O4	PROTO-PORPHYRIN
5760	DIETHYL ETHER	517	19	-0.32		C34H38N4O6	HEMATO-PORPHYRIN
5761	DIETHYL ETHER	517	19	0.52		C34H38N4O6	MESO-PORPHYRIN
5762	DIETHYL ETHER	359		0.85	1.62 B	C34H47N1O11	ACONITINE
5763	CHCL3	359		1.77	1.28 B	C34H47N1O11	ACONITINE
5764	OCTANE	57		-0.15		C34H62O11	P-T-OCTYLPHENOXYNONAETHOXYETHANOL/OPE-9/
5765	DIETHYL ETHER	518		1.09	1.08 A	C35H36N2O6	MONODEMETHYL-L-CURINE
5766	OCTANOL	519		1.79	1.79 =	C35H61N3O14	3-AZIDO-3'-DE(DIMEAMINO)-4'-HYDROXYERYTHROMYCIN
5767	DIETHYL ETHER	518		0.15	0.25 A	C36H38N2O6	D-CHONDROCURINE
5768	DIETHYL ETHER	517	19	-0.48		C36H38N4O8	COPRO-PORPHYRIN
5769	OCTANOL	519		2.21	2.21 =	C36H65N1O13	N-DESMETHYLERYTHROMYCIN
5770	OCTANOL	519		1.26	1.26 =	C36H65N1O13	ERYTHROMYCIN C
5771	OCTANE	57		-0.59		C36H66O12	P-T-OCTYLPHENOXYDECAETHOXYETHANOL/OPE-10/
5772	OCTANOL	519		3.12	3.12 =	C37H67N1O12	DEOXYERYTHROMYCIN
5773	DIETHYL ETHER	519	50	1.59	1.52 A	C37H67N1O12	DEOXYERYTHROMYCIN
5774	CYCLOHEXANE	519		0.39		C37H67N1O12	DEOXYERYTHROMYCIN
5775	CHCL3	519		2.64	3.08 N	C37H67N1O12	DEOXYERYTHROMYCIN
5776	BENZENE	519		2.18	3.50 A	C37H67N1O12	DEOXYERYTHROMYCIN
5777	TOLUENE	519		1.86	3.21 A	C37H67N1O12	DEOXYERYTHROMYCIN
5778	ETHYL ACETATE	519	50	1.62	1.78	C37H67N1O12	DEOXYERYTHROMYCIN
5779	1-PENT. ACETATE	519	50	1.90	1.79	C37H67N1O12	DEOXYERYTHROMYCIN
5780	CCL4	519		1.36	2.63 N	C37H67N1O12	DEOXYERYTHROMYCIN
5781	DI-I-PR. ETHER	519	50	1.07	1.78	C37H67N1O12	DEOXYERYTHROMYCIN
5782	ME-I-BUT.KETONE	519	50	1.30	1.25	C37H67N1O12	DEOXYERYTHROMYCIN
5783	OCTANOL	519		2.48	2.48 =	C37H67N1O13	ERYTHROMYCIN
5784	DIETHYL ETHER	519	50	1.30	1.26 A	C37H67N1O13	ERYTHROMYCIN
5785	CYCLOHEXANE	519		-0.22		C37H67N1O13	ERYTHROMYCIN
5786	CHCL3	519		2.46	2.90 N	C37H67N1O13	ERYTHROMYCIN
5787	BENZENE	519		1.62	2.94 A	C37H67N1O13	ERYTHROMYCIN
5788	TOLUENE	519		1.45	2.85 A	C37H67N1O13	ERYTHROMYCIN
5789	ETHYL ACETATE	519	50	1.28	1.43	C37H67N1O13	ERYTHROMYCIN
5790	CCL4	519		1.25	2.93 A	C37H67N1O13	ERYTHROMYCIN
5791	DI-I-PR. ETHER	519	50	0.63	1.28	C37H67N1O13	ERYTHROMYCIN
5792	ME-I-BUT.KETONE	519	50	1.16	1.16	C37H67N1O13	ERYTHROMYCIN
5793	OCTANOL	519		1.44	1.44 =	C37H67N1O14	4'-HYDROXYERYTHROMYCIN
5794	OCTANOL	65	56	-2.18	-2.18 =	C38H42N2O6	O-TETRANDRINE/NCS-77037/
5795	OCTANOL	519	55	3.11	3.11 =	C38H65N1O14	ERYTHROMYCIN-9,11-CARBONATE-6,9-HEMIKETAL
5796	TOLUENE	148		2.44	2.44 B	C39H33FE1N12O3	FERRIC-CARBAZONE COMPLEX
5797	OCTANOL	519		3.32	3.32 =	C39H69N1O13	11-O-ACETYLDEOXYERYTHROMYCIN
5798	OCTANOL	226	54	-1.27	-1.27 =	C41H48N2O8	THALICARPINE (68075)
5799	I-BUTANOL	130		1.59	1.73	C41H64O13	DIGITOXIN
5800	OCTANOL	65	46	-1.60	-1.60 =	C43H43N7O7S2	NCS-114347

NO.	SOLVENT	REF	FOOT NOTE	LOGP SOLV	LOGP OCT	EMPIRICAL FORMULA	NAME
5801	OCTANOL	227		2.82	2.82 =	C46H56N4010.H2S104	VINCRISTINE SULFATE (PKA= 5.5)(NCS 67574)
5802	OCTANOL	227		3.72	3.72 =	C46H58N409.H2S104	VINCALEUKOBLASTINE SULFATE (PKA= 5.4)(49842)
58C3	SEC-BUTANOL	84	19	1.21	1.19	C60H92N12010	GRAMICIDIN S-A
5804	SEC-BUTANOL	84	19	-0.07	-0.63	C66H103N17016S1	BACITRACIN A
58C5	SEC-BUTANOL	84	19	-1.08	-2.28	C999	INSULIN
58C6	SEC-BUTANOL	84	19	0.51	0.21	C999	POLYPETIN A

[1] pH 1.1, 37°. [2] At pH = pI net charge = zero. [3] In *n*-pentyl acetate. [4] Calculated $\log P_{enol} = 1.48$; $\log P_{keto} = 0.04$; intramolecular H bonds indicated. [5] P reported constant between pH 2 and 6. [6] No $\log P_{oct}$ values were calculated because the H-bonding capabilities of boronic acids were greatly influenced by the σ constant of substituents. [7] pH 2.0. [8] The large difference between the 3 and 4 isomers is explained in ref 478. [9] Compounds with active hydrogens show unusually high $\log P_{benzene}$ values. [10] At pH 7.4 plus hexadecylamine; the addition compound is also partitioning. [11] Some lactone also present. [12] This value appears "out of line"; it was not used in the regression equation. [13] $P_{un\text{-}ionized} = P^*/(1 - \alpha)$, where α = degree of dissociation calculated from pK_a. [14] pH 7.4 + phosphate buffer; not ion-corrected. [15] pH 3.5. [16] pH ~1.0. [17] Apparent P reported; not buffered or ion-corrected. [18] pH 7.05 + octadecylamine; addition compound is also partitioning. [19] pH 1.0 using HCl. [20] pH −0.22 using HCl. [21] pH 7.1 + octadecylamine; addition compound also partitioning. [22] Value is ratio of solubilities, not a true P, but the activity of an inert gas is nearly unity even at saturation. [23] pH 7.3; ion-corrected [24] pH 7.3; estimated pK_a = 4.9; absolute values not very reliable but comparison within series valid. [25] Corrected for ionization and dimerization by method of ref 29. [26] Approximate value. [27] pH 7.3 in ref 489; pH 7.0 in ref 206; both ion-corrected. [28] pH 6.3, ion-corrected. [29] pH 5.9. [30] pH 6.9. [31] pH 7.4; ion-corrected from pK_a. Absolute values not reliable, but comparison within series valid. [32] pH 5.4. [33] pH 7.8. [34] pH 6.0. [35] pH 7.1. [36] pH 6.5 using 1 *M* phosphate buffer; method = countercurrent extraction. [37] pH 7.1 using 0.1 *M* phosphate + 1 *M* NaCl. [38] pH 6.6 + 1 *M* phosphate. [39] pH 6.9 using phosphate buffer. [40] pH 5.6 using phosphate buffer; ref 504 also lists values at pH 2.1–8.5. [41] This reference also lists values for decyl, undecyl, and dodecyl ion pairs. [42] May be dimerized in organic phase. [43] pH 7.5 + 0.2 *M* phosphate. [44] pH 7.4 using phosphate buffer, ion-corrected. [45] Calculated from the mole fraction partition coefficient (P_{MF}) by the expression $P = (P_{MF}) \times 18(do)/MW_o$, where do = density of organic solvent and MW_o = its molecular weight. [46] Ion pair. [47] Calculated from ratio $C_w/(C_o)^{1/2}$ and the K_{dimer} from ref 139. [48] At isoelectric point, pH 5.35. [49] pH 5.8; ion-corrected using pK_a = 4.8. [50] Classification by regression equation appears anomalous. [51] 0°. [52] Aqueous phase is 5% HCl. [53] In plastic containers. In alkylpyridinium series, adsorbtion to glass gives values lower by 0.15 (decyl), 0.3 (hexyl), and 0.8 (butyl). [54] Dissolved in HCl, adjusted to pH 6.5. [55] Subject of U. S. Patent 3,417,077 issued to Eli Lilly & Co. [56] pH 4.0. [57] pH 8.0 using 0.02 *M* phosphate-citrate buffer. [58] Assay procedure: *J. Agr. Food Chem.*, **8**, 460 (1960). [59] Commercial material: 96% pure. [60] pH 11 using Sorenson's buffer. [61] pH 4.7; $\log P^* = -2.00$ at pH 2.2. [62] Calculated as $\log P = (pE + 2) - pK_a$. [63] pH 6.4, ion-corrected. Log P's calculated from π values listed and $\log P_{CHCl_3} = -1.40$ and $\log P_{oct} = -0.70$ for sulfanilamide. [64] pH 5.5; phosphate buffer; largely as anion; some polymer possible. [65] pH 7.4 using phosphate buffer; *not* ion-corrected. [66] pH 8.93 using carbonate buffer; ion-corrected. [67] pH 9.2 using carbonate–bicarbonate buffer; ion-corrected. [68] pH 1.0; approximately half of phenothiazine ring nitrogens protonated. [69] pH 7.6; where solute has two alkyl N atoms, some diprotonation probable. [70] Entered twice: once as enol, once as keto tautomer. [71] pH 12.8; *not* ion-corrected; ~0.0001% in neutral form. [72] pH 7.32; *not* ion-corrected; ~0.1% in neutral form. [73] pH 10.15 using carbonate–bicarbonate buffer. [74] pH 13.7; *not* ion-corrected; ~0.01% in neutral form. [75] pK_a measured in acetonitrile which accentuates base strength. [77] Log P at infinite dilution calculated by regression analysis; $s = 0.03$, $r = 0.995$. Note: mixed solvent #1 is 67% (by volume) ethyl ether and 33% petroleum ether.

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