Octanol-Water Partition Coefficients of Simple Organic Compounds

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Octanol-water partition coefficients (log P) for 611 simple organic compounds representing all principal classes have been retrieved from the literature. Available experimental details of measurement are documented from original articles. Pertinent thermodynamic relations are presented, with a discussion of direct and indirect methods of measurement. Reported log P data for each compound have been evaluated according to stated criteria, and recommended values (with uncertainty) are given.

Key words: octanol-water partition coefficient; organic compounds; hydrophobicity; hydrophilicity

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List of Symbols and Abbreviations

a = activity
AMB = ambient temperature
AQ = octanol-saturated water phase
AS = absorption spectrophotometry
B = organic base
c = concentration
C_p = heat capacity at constant pressure
CR = chemical reaction
D = direct method
FL = fluorescence
G = Gibbs energy

GC = generator column
GLC = gas-liquid chromatography
h = chromatographic peak height, Eq. (28)
H = enthalpy
HA = organic acid
H_M = Henry's law constant
(RP)-HPLC = (reverse-phase) high pressure liquid chromatography
I = indirect method
K = Kjeldahl method
K_a = acid ionization constant
l = liquid
m,n = correlation constants, Eq. (10)
NS = neutral salt solution
ORG = water-saturated octanol phase
p = pressure
P = partition coefficient
P_{app} = apparent partition coefficient
RC = radiochemical method
s = solid
S = entropy
SF = shake-flask method
T = temperature (kelvin)
Temp. = temperature of log P measurement (°C)
TN = titration
v = volume (general)
V = molar volume (L mol^{-1})
W = octanol-saturated water solvent
x = mole fraction
X = solute
? = doubtful Log P value; Code uncertain

Greek
Δ = difference in thermodynamic function
γ = volume-fraction activity coefficient
μ = chemical potential
φ = volume fraction
ζ = solubility (mol L^{-1})

Superscripts
aq = octanol-saturated water phase
0 = standard state
oct = pure octanol phase
org = water-saturated octanol phase
sat = phase saturated with solute
w = pure water phase
* = Hansch & Leo "selected" Log P value

Subscripts
app = apparent (partition coefficient)
fus = fusion
f = final
i = initial
org = water-saturated octanol phase
tr = transfer process
X = solute

1. Introduction

1.1. General

1.1.a. Definition

A pure substance may distribute itself between two partially miscible solvents in intimate contact, and the equilibrium ratio of solute concentrations in the two phases has come to be known as the distribution coefficient or partition coefficient.[1] In preparative organic chemistry, the use of solvents of greatly differing polarity (e.g., hydrocarbon and water) facilitates the extraction and purification of desired products. In addition, the biological activity of simple organic compounds was early found to correlate with their oil-water partition coefficients.[2] It became apparent that, for biological purposes a partition coefficient based on long-chain ester or alcohol solvents was more appropriate. After some deliberation, 1-octanol was chosen as the most useful lipophile solvent in these applications. Most correlation work has been done using the octanol-water pair, and this is the reason for its wide use and the existence of a great quantity of data on the subject.

The octanol-water partition coefficient of a substance X at a given temperature is, by general consent,[1] represented by P and defined by (for reasons explained later, the superscripts "org" and "aq" are used to denote mutually saturated phases, and "oct" and "w" for the pure solvents.)

$$P = [X]^{\text{org}}/[X]^{\text{aq}}, \tag{1}$$

i.e., the ratio of concentrations (mole/volume) at equilibrium; it is therefore unitless. In the interest of standardization and precision in interpretation, the partition coefficient is defined for the same species on both phases.[1] This is important in considering P of ionizable compounds such as organic acids, amines, and quaternary ammonium salts, which may also form dimers or ion-pairs. This is discussed further in this Introduction.

In addition, the solvents represented in Eq. (1) are those mutually saturated with each other at the temperature of measurement. This is a natural consequence of the classical "shake-flask" or extraction method used in experimental measurement of P, and is to be taken into account for accuracy in measurement and thermodynamic interpretation.

Further, P is preferably defined as the quantity which is independent of concentration, i.e., that value for which the solute obeys Henry's law in both solvents simultaneously. In practice, this means a P determined at high dilution, or extrapolated to zero concentration. Since P as measured can range over many orders of magnitude (10^{-2} to 10^{6}), it is usually expressed as its decadic logarithm, log P.

1.1.b. Scope of this evaluation

This work proposes to have retrieved and evaluated most of the significant published experimentally determined values of log P of simple organic molecules. The word "simple" is taken here to indicate molecules containing no or only one polar functional group, i.e., a group having N,O,S and/or halogen atom. A few well-known exceptions (chloroform, CCl_4) have been included. This limits the number of substances involved and, as far as possible, avoids complications of interpretation due to the presence of neighboring polar groups. The compounds are those which are liquids or solids at ordinary temperatures and pressures, and no arbitrary upper carbon number cutoff limit has been imposed. Elements, inorganic, metal-organic and unstable species have been excluded, as well as quaternary ammonium and similar salts.

1.1.c. Need for critical evaluation

The partition coefficient, as properly defined, is a definite equilibrium physico-chemical property of a pure substance under specified conditions. It provides a useful quantitative parameter for representing the lipophilic/hydrophilic nature of the substance. It is a function of the Gibbs energy of transfer from water to octanol and hence describes the thermodynamic tendency for the compound to partition preferentially in different media. It is not surprising, therefore, that it has been widely used in many areas such as:

- -design of drugs and pharmaceuticals,[4]
- -prediction and correlation of bioconcentration[5] and soil and sediment sorption of organic pollutants,
- -research on medicinal chemicals,
- -modelling of environmental fate of organic chemicals,[6]
- -toxicology of substances.

For many substances, log *P* has been measured by different laboratories and by different methods. The reported log *P* values of a single substance can sometimes vary a great deal; for example, those of *p,p'*-DDT cover a range of a factor of one hundred.[2] Large uncertainties in log *P* are undesirable in general. The accuracy of the simulation, by calculation, of the environmental fate of an organic chemical may become quite sensitive to uncertainties of input parameters (e.g., Mirex in Lake Ontario[7]). The successful development of additive-constitutive calculational schemes[2,8] for log *P*, based on molecular structure, requires a database of assessed accuracy. Finally, it is difficult, if not impossible, for the uninitiated user of log *P* data to distinguish accurate and inaccurate data by simple inspection.

1.2 Thermodynamics

The thermodynamic relationships between log *P* and other quantities will be examined in some detail in this section. Many experimental data on log *P* related thermodynamic quantities have appeared recently, some of high quality. Since these were not discussed in any detail in former compilations and reviews,[1,2] the following exposition is meant to summarize the important thermodynamic relations in a concise and rigorous manner.

1.2.a. General equilibrium relations

The present thermodynamic analysis is a slightly edited restatement of the one currently being used to describe the two-phase system represented by the octanol-water partition coefficient.[9,10,34,38,58] Like the current practice, it uses volume fractions as composition variable and volume fraction activity coefficients. This convention, when used in conjunction with the (volume-based) partition coefficient, simplifies the thermodynamic argument. An equivalent though incomplete, analysis using mole fractions is given elsewhere.[33,39] If a liquid substance *X* is distributed between organic and aqueous phases at equilibrium, we can write for each phase[9]

$$\mu_X = \mu_X^0 + RT \ln a_X \tag{2}$$

$$= \mu_X^0 + RT \ln(\gamma_X \varphi_X), \tag{3}$$

where μ_X is the chemical potential of *X* in solution, μ_X^0 is the chemical potential of pure liquid *X*, a_X is its activity in solution, γ_X is the volume-fraction activity coefficient and φ_X is the volume fraction of *X* in the solution. From the defining Eqs. (2) and (3), the activity coefficient is normalized by $\gamma_X \to 1$ as $\varphi_X \to 1$.

By definition, in each phase we have

$$[X] V_X = \varphi_X, \tag{4}$$

where V_X is the (partial) molar volume of *X* in solution. (For dilute solutions of liquid nonelectrolytes in water or octanol, partial molar volume can be replaced by pure liquid molar volume without appreciable error.) At equilibrium, $\mu_X^{\text{org}} = \mu_X^{\text{aq}}$. Combining this equality with Eqs. (1), (3), and (4) yields[9]

$$\log P = \log(\gamma_X^{\text{aq}} / \gamma_X^{\text{org}}), \tag{5}$$

i.e., *P* is equivalent to the ratio of the Henrian activity coefficients of the solute in the phases. Equation (5) has been derived using the assumption that $V_X^{\text{aq}} = V_X^{\text{org}}$.

1.2.b. Temperature dependence

The variation of log *P* with temperature[1] is small, approximately $\pm 0.01\ \text{K}^{-1}$. Table 1 presents experimental data of $d(\log P)/dT$ for some specific compounds.

The thermodynamic transfer functions are closely related to log *P*:

$$\Delta_{\text{tr}} G = -RT \ln P \tag{6}$$

$$d(\Delta_{\text{tr}} G)/dt = -\Delta_{\text{tr}} S \tag{7}$$

$$\Delta_{\text{tr}} G = \Delta_{\text{tr}} H - T \Delta_{\text{tr}} S \tag{8}$$

As a consequence of the definition of *P*, these transfer quantities are independent of concentration and refer to the difference: (function for solute in water-saturated octanol)—(function for solute in octanol-saturated water).

The temperature dependence of $\Delta_{\text{tr}} G$ and hence of log *P* can be represented by $\Delta_{\text{tr}} H$ and $\Delta_{\text{tr}} S$ through Eqs. (6), (7), and (8). A van't Hoff plot of ln *P* may be used to obtain

TABLE 1. Temperature dependence of Log *P* of some compounds at room temperature

Substances	Temperature range, °C	1000 $d(\text{Log } P)/dT$ K^{-1}	Ref.
n-propylbenzene	10–35	≈0	10,11
chlorinated benzenes	13–33	− 29 to − 5	12
phenol	10–60	− 3.4	16
phenol	20–50	− 4.9	17
p-cresol	15–35	− 7.5	18
phenol	15–35	− 16	18
m-alkoxyphenols	15–35	− 5 to − 3	19
resorcinol	15–35	− 8.8	19
substituted phenols	10–60	− 8 to − 1	16
substituted phenols	20–50	− 3 to + 10	17
chlorophenols	···	− 8.6 (mean)	20
hydroxybenzoic acids	···	− 14 (mean)	20
methyl nicotinate	5–25	7.4	14
ephedrine	15–40	8.1	15
methamphetamine	15–40	0.4	15
alkyl amidylpyridines	20–40	2 to 6	13
methyl acetanilides	···	≈0 (mean)	20

enthalpy and entropy of transfer.[17-20] However, P is a Gibbs energy function—as are solubility and vapor-liquid equilibrium—and these functions are usually found to be relatively insensitive to temperature. The enthalpy of transfer may be more precisely determined[21] either by direct experimental measurement in an isoperibol flow calorimeter[22,23] (in which two immiscible phases are brought into direct contact) or indirectly from the calorimetric limiting enthalpies of solution in the two solvents separately.

As will be discussed in greater detail in the next section, both $\Delta_{tr}G$ and $\Delta_{tr}H$ may be determined from measurements on solutions based on the two solvents separately. This is a possible route, provided it is realized that solute thermodynamic functions in pure water or pure octanol may be significantly different from those in mutually saturated solvents.

1.2.c. Specific thermodynamic relations

Mutually saturated solvents.

From liquid–liquid equilibrium data[2,4] the equilibrium mole fractions of octanol in the two-phase system water/*n*-octanol at 25 °C are 7.03×10^{-5} and 0.793. Saturated octanol thus contains an appreciable amount of water; the molar volume of wet octanol[25] is 126.6 cm^3, and the water content is equivalent to 1.64 mol L^{-1}. The two phases in a shake-flask determination of P are ternary. The question whether or not the presence of the other solvent in a phase significantly alters the thermodynamic properties of the solute becomes important in considering recently elaborated "activity coefficient" methods of determining the partition coefficient.

For example, Berti *et al.*[22] compared the transfer Gibbs energies from shake-flask log P values of some common solutes to those found from the directly measured Henrian activity coefficients of the same solutes in pure octanol and pure water. The differences in $\Delta_{tr}G$, 1 to 2 kJ mol^{-1}, is equivalent to differences of as much as ± 0.4 in log P, being negative or positive or zero, depending on the solute. Calorimetrically determined enthalpies of transfer of *m*-alkoxy phenols[26] in neat and mutually saturated solvents differed by up to 1.6 kJ mol^{-1}; the same effect is found in the corresponding enthalpies of solution[22,26] from which the transfer enthalpies are derived. Again, the magnitude of the effect depends on the solute; the transfer enthalpies of *n*-alkanols[27] for example, are much less sensitive in this respect.

Platford[28,29] used the isopiestic method to measure the limiting activity coefficients of CCl_4 and benzene in neat and mutually saturated solvents, and found no detectable difference in the results. Henrian activity coefficients in octanol for 22 monofunctional compounds were measured by gas chromatography[58]; within experimental error the relation

$$P=\gamma_X^{w}/\gamma_X^{oct}, \tag{9}$$

was valid.

Relationship with aqueous solubility.

Thermodynamic considerations have also elucidated the relation between log P and aqueous solubility, ζ, early proposed by Hansch et al.[30] Since both log P and ζ may be regarded as Gibbs energy transfer functions, an equation of the type

$$\log P = m\log\zeta + n, \tag{10}$$

might be expected to be valid, where m and n are correlation coefficients. A relation like Eq. (10), if true, would greatly reduce the experimental effort necessary to obtain P. The search for refinement and rationalization of Eq. (10) has been lively, giving rise to at least one polemic exchange in the literature.[31,32]

A relation of the form of Eq. (10) can be derived from thermodynamic first principles.[33,34] The case for a liquid solute will be given first, as a solid solute introduces a complication into the argument. For a liquid solute distributed at equilibrium between organic and aqueous solvents (The solvents are assumed to be mutually saturated, in order to keep the analysis as close as possible to the conditions in a real shake-flask situation.) Eq. (3) can be applied to both phases to give

$$(\gamma_X\varphi_X)^{org}=(\gamma_X\varphi_X)^{aq} \tag{11}$$

which, by Eq. (4) becomes

$$(\gamma_X[X])^{org}=(\gamma_X[X])^{aq}. \tag{12}$$

Consider now, as a separate system, the solute in saturation equilibrium in the aqueous solvent. On the assumption that the equilibrium free solute contains no solvent, Eq. (3) under these conditions becomes

$$\mu_X=\mu_X^0=\mu_X^0+RT\ln(\gamma_X\varphi_X)^{sat} \tag{13}$$

or

$$(\gamma_X\varphi_X)^{sat}=1. \tag{14}$$

Combined with Eq. (4), this becomes

$$(\gamma_X c_X V_X)^{sat}=1, \tag{15}$$

where c_X has units inverse to that of V_X. Recalling Eqs. (1) and (5),

$$P=[X]^{org}/[X]^{aq}=\gamma_X^{aq}/\gamma_X^{org}. \tag{16}$$

Introducing Eq. (15),

$$P=1/(\gamma_X^{org}\zeta_X^{aq}V_X) \tag{17}$$

$$\log P = -\log\zeta_X-\log(\gamma_X V_X)^{org}, \tag{18}$$

Eq. (18) has the same form of Eq. (10). Clearly, data for liquid solutes would all fall on a common linear plot of log P vs log ζ, with the following provisos:

ASSUMPTION 1: γ_X^{org}, the Henrian activity coefficient for liquid solutes in organic solvent, is the same for all solutes.
ASSUMPTION 2: ζ_X refers to water saturated with octanol.
ASSUMPTION 3: the solute obeys Henry's law for concentrations up to saturation in the aqueous solvent.
ASSUMPTION 4: the free liquid solute, as an equilibrium phase, contains no solvent (i.e., its activity is unity).

For solutes which are solid at temperature of measurement, fundamental equations such as Eq. (2) are valid. In this case, however, the reference state for μ_X^0 cannot be the pure solid, since it is desirable to keep the same Raoult's law convention for the activity coefficients. The approach is then through solid–liquid equilibrium. For a component in equilibrium between solid and liquid phases,

$$\mu_X(s) = \mu_X(1), \tag{19}$$

$$\mu_X^0(s) + RT\ln a_X(s) = \mu_X^0(1) + RT\ln a_X(1), \tag{20}$$

$$\mu_X^0(1) - \mu_X^0(s) = RT\ln a_X(s)/a_X(1). \tag{21}$$

The quantity on the left-hand side of Eq. (21) is the Gibbs energy of fusion of the solute at temperature T, $\Delta_{\rm fus}G_T^0$. If the equilibrium solid phase is pure solid, then

$$\Delta_{\rm fus}G_T^0 = -RT\ln a_X(1). \tag{22}$$

For temperatures below the normal melting point of the solute, $\Delta_{\rm fus}G_T^0$ refers to the process (solid → supercooled liquid).[34,35] Since the solution is saturated,

$$\Delta_{\rm fus}G_T^0 = -RT\ln(\gamma_X\varphi_X)^{\rm sat}. \tag{23}$$

The thermodynamic argument represented by Eqs. (12)–(18) can be repeated again, with Eq. (23). The result is

$$\log P = -\Delta_{\rm fus}G_T^0/2.303RT - \log\xi_X - \log(\gamma_X V_X)^{\rm org}, \tag{24}$$

Eq. (24) is the same as Eq. (18), with the addition of the Gibbs energy of fusion term. The validity of Eq. (24) is of course subject to the same assumptions attached to Eq. (18).

For correlation purposes, the Gibbs energy of fusion to the supercooled liquid state may be expressed in terms of the usual fusion quantities:

$$\begin{aligned}-\Delta_{\rm fus}G_T^0/RT &= (\Delta_{\rm fus}H^0/2.303R)(T - T_{\rm fus})/TT_{\rm fus} \\ &\quad + (\Delta_{\rm fus}C_p^0)(\ln(T/T_{\rm fus}) + (T_{\rm fus} - T)/T).\end{aligned} \tag{25}$$

In Eq. (25), the enthalpy and heat capacity quantities refer to corresponding changes at the normal melting point ($T_{\rm fus}$). [The heat capacities of solid and liquid solute have been assumed to be independent of temperature. They are not so in general, and Eq. (25) could be modified to take this into account.] Eqs. (24) and (25) together are identical to Eq. (14) of Miller *et al.*[34] Eq. (25) may be simplified by putting $\Delta_{\rm fus}C_p^0 = 0$ and[36] $\Delta_{\rm fus}H^0 = T_{\rm fus}\,\Delta_{\rm fus}S^0 = 56.5T_{\rm fus}$ J mol^{-1}. The result is an expression equivalent to Eq. (26) of Mackay *et al.*[33]

Apart from these simplifications, the four assumptions quoted above are of varying importance. The Henrian activity coefficient in octanol, $\gamma_X^{\rm oct}$, has been estimated by indirect[33] and direct[37,38] methods. It is clear, particularly for hydrophobic compounds, that this activity coefficient increases with molecular weight (or molar volume). The water solubility ξ_X is usually taken as that in pure water. The solubilities of organic compounds in octanol-saturated water are measurably different.[26,38,39] The difference increases with molecular weight. It is difficult at present (if not impossible) to define precisely the individual errors introduced into Eqs. (18) and (24) by these assumptions and simplifications.[33,38,39]

Ratio of solubilities.

It has been stated that P is equivalent to the ratio of solute solubilities in the two solvents,[40] or is well approximated by this ratio.[37] The thermodynamic justification for liquid and solid solutes is derived from Eqs. (1), (15), and (22) for the case of two phases saturated with solute. The result is

$$P = \xi_X^{\rm org}/\xi_X^{\rm aq} \approx \xi_X^{\rm oct}/\xi_X^{w} \tag{26}$$

As before, the important qualifying assumptions apply here also. There may be some fortuitous cancellation of effects. Yalkowsky *et al.*[37] have tested Eq. (26) using solubilities in neat solvents for 36 solid compounds and found reasonable, though not exact, correlation.

Henry's law.

The Henry's law constant, like log P, is a limiting Gibbs energy quantity and its usefulness overlaps that of log P.[41] Henry's constant for a solute on the mole fraction scale, H_M, may be defined as[41] (where x is the mole fraction of solute)

$$\lim_{x\to 0}(p/x) = H_M, \tag{27}$$

where p is the partial pressure of solute above the solution. Henrian behavior of solutes has been exploited[42] in the "head-space gas chromatographic method" for measuring P. The principal feature of this method[43] is the sampling and quantitative analysis, by gas chromatography, of the vapor mixture above a liquid solution. In a measurement of P, the vapor above an unsaturated aqueous solution (volume v_1) of the solute is sampled and the gas chromatographic peak height (h_1) of the solute is obtained. A volume v_2 of octanol is added, and after equilibration the vapor is sampled and analyzed as before (h_2). The partition coefficient is then

$$P = v_1(h_1/h_2 - 1)/v_2. \tag{28}$$

Equation (28) assumes that Henry's law is obeyed by the solute in the aqueous phase; that H_M is independent of the presence of co-solvent; that there is a strict mass balance for the solute; and the vapor behaves ideally.

1.3. The case of ionizable solutes

In the present work, two types of organic compounds may ionize in aqueous solution, viz., acids (HA) and amines (B):

$$\mathrm{HA} \rightleftharpoons \mathrm{H^+} + \mathrm{A^-}, \tag{29}$$

$$\mathrm{BH^+} \rightleftharpoons \mathrm{B} + \mathrm{H^+}, \tag{30}$$

where A^- is the acid anion. [Water should appear on both sides of Eqs. (29) and (30), but since in dilute solution its activity is practically unity and does not change, it may be omitted from the thermodynamic analysis.] The thermodynamic dissociation constant isdefined as

$$K_a = a(\mathrm{H^+})a(\mathrm{A^-})/a(\mathrm{HA}) \tag{31}$$

after Eq. (29), and

$$K_a = a(\mathrm{H^+})a(\mathrm{B})/a(\mathrm{BH^+}) \tag{32}$$

after Eq. (30). Since P is defined only for the same (undissociated) species in both phases, the *apparent* partition coefficient $P_{\rm app}$ (sometimes called distribution coefficient) measured in the presence of appreciable ionization according to Eqs. (29) and (30) will differ from P. It can be shown[44] that $P_{\rm app}$ and P for an acid are related by

$$P = P_{\rm app}[1 + 10^{(pH - pK_a)}] \tag{33}$$

and for an amine by

$$P = P_{\mathrm{app}}\,[1 + 10^{(pK_a - pH)}]. \tag{34}$$

For weak acids ($pK_a \gg 7$) or weak bases ($pK_a \ll 7$) in water, there is negligible ionization ($P_{\mathrm{app}} = P$). For other compounds under some experimental conditions, there will be appreciable ionization. [For example, phenol is a very weak acid ($pK_a = 9.9$) and is not appreciably ionized in neutral solution. For pentachlorophenol, however, the alcoholic hydrogen atom is rendered more labile ($pK_a = 4.8$). The measured values of P over the pH range 1.2–13.5 vary by more than three orders of magnitude.[45]] In these cases, P_{app} may be corrected according to Eqs. (33) and (34), or a buffer of suitable pH may be used as the aqueous phase in order to suppress ionization. Some compounds (e.g., acids) may form dimers or other associated species in the organic phase. This source of error may be avoided by the use of sufficiently dilute solutions, which is usual practice.

2. Methods of Measurement

Values of P reported in the literature have been determined by many methods. Mention is made in this section of a rather large number of these, but only the more reliable or soundly based will be discussed in some detail. For the purposes of evaluation, the methods have been classified into two groups (direct and indirect). This division is made for convenience of discussion, and does not necessarily imply fundamental or far-reaching theoretical differences.

2.1. Direct or "experimental" methods

2.1.a. Shake-flask method

This classic extraction procedure is widely used and, with due attention to experimental conditions, manipulation and range of applicability produces reliable results. It has been described briefly[46] and necessary precautions have been discussed in some detail.[1,3] The case of weakly ionized solutes has been given special attention.[47] In essence, the method is simple. A small amount of the solute is dissolved in either aqueous or organic phase, equilibrium partition is obtained by agitation, the phases are separated and one or both phases are analyzed for solute. Apart from requirements already mentioned in Sec. 1 of this review, a few of the other important precautions may be mentioned here.

Purity of chemicals.

Depending on the analytical method used, the presence of partitionable impurities in solvents or sample may lead to erroneous measured solute concentrations.

Mutually saturated solvents.

It is often the practice in this method to prepare a solution of known initial solute concentration c_i in one solvent, and equilibrate a definite volume v_1 of this with a definite volume v_2 of the other solvent. The final solute concentration c_f is measured in the first solvent and the partition coefficient is given by the ratio $(c_i - c_f)v_1/c_fv_2$ or its inverse. Since the densities of neat octanol and water-saturated octanol are measurably different, the use of presaturated solvents avoids any error through changes in solvent volume upon equilibration.

Mixing and separation.

Several different methods of agitation are used to
the solvents into intimate contact. In general, prolong
violent shaking is not necessary and tends to cause em
formation. The phases separate under normal gravit
they are usually centrifuged to accelerate the separati
the smallest droplets.

Sampling.

Ideally, both phases are analyzed. This is not a
done, for reasons of convenience and time. If only one
is analyzed, a mass balance between the phases is ass
and it must be established that no solute has been l
adsorption on glass, rubber stopper or other material u
manipulation. Since many solutes preferentially par
into the organic phase, care must be taken to ensur
sampling devices introduced into the phases do not ina
tently carry over one phase into the other.

Analysis.

Absorption spectrophotometry and gas–liquid
matography are often used. There may be intermedia
traction and/or concentration steps, or one involv
chemical reaction. The usual precautions in quanti
analysis apply here.

Volatile solutes.

If the solute has an appreciable vapor pressure it m
necessary to consider the amount of vapor space in the
libration vessel and details of manipulation during sam
analysis, etc.

Since the shake-flask method is at times tediou
time-consuming, a number of automated or simplifie
sions have been used. Most are closed-loop flow devic

-counter-current distribution (engineering de
Centrifugal partition chromatography[49] may b
scribed as the addition of a high gravity field t
counter-current method.

-The AKUFVE system[50] uses continuous centri
tion to separate the phases, while the rapid mix
probe[51,52] uses different membrane filters.

-the segmented flow device[53] is a miniaturized co
current flow system.

-a three-phase partition system[54] is a kind of co
current method using two aqueous phases:

$$AQ_1/ORG/AQ_2,$$

where AQ_1 and AQ_2 are different aqueous b
This device is used principally for investigating
ics of partition.

-the exponential concentration change method[55]
be regarded as a multi-step extraction procedure

2.1.b. Generator column method

The ordinary liquid chromatographic column
has been adapted for the measurement of partition
cients.[10,11] The solid support is usually silanized dia
ceous silica. The column is loaded by pulling an unsatu
solution of the solute of interest at a known concentrat
water-saturated octanol through the column. The sol
eluted with octanol-saturated water, and the effluent i
lyzed by high pressure liquid chromatography or gas–

omatography. A primary advantage of this design[10] is the ence of any possibility of emulsion formation, since the ents are brought into intimate contact by slow permea- of one through the other. It is a closed system and ma- ulation is minimized; it is a flow system and so interior faces in contact with solute in solution may be "condi- ed", if necessary, without affecting accuracy.

2.2. Indirect or "Calculation/Correlation" Methods

a. Methods widely used and/or having some theoretical justification

The deduction of P from aqueous solubility and Hen- law constants has been discussed in Sec. 1.2.c. Probably most widely used correlation method is that with solute ention volumes or chromatographic capacity factors in ersed-phase high pressure liquid chromatography (RP- LC).[56–58] The possibility of obtaining a single general pose correlation has been extremely seductive, as evi- ced by the large number of published attempts and de- ed investigation of the interacting effects among solute arity, eluent composition and chemical nature of the sta- ary phase.[59] The attempt cannot be described as totally cessful, despite recent refinements such as coating the ionary phase with octanol[60–62] or dipalmitoyl phosphati- choline[63] and use of ω-hydroxy silica[64] as column pack- . It appears that satisfactorily precise correlations are ob- ed when the results are extrapolated to 100% water as ent or when homologous series plots are used.[58,65] The thod is easily automated.[66]

Reverse-phase thin layer chromatography (RP- C)[67,68] may be considered the two-dimensional analogue P-HPLC. The precision of RP-TLC, including a chemi- y modified version,[69] is generally inferior to RP-HPLC.

For weakly ionizable solutes, a potentiometric titration thod has been used.[70] Sometimes called microelectrome- titration, this procedure yields values for both P and K_a single experiment. Equations have been given for difunc- al acids[71] and a completely automated version has been cribed.[44] An analogous thermometric titration proce- e, based on the enthalpy of protonation of an amine, has been used.[72]

A statistical analysis for a correlation between loga- ms of octanol-water and cyclohexane-water partition co- cients was carried out by Seiler[73] for 230 compounds. A ar relation was found, and the intercept included a term resenting hydrogen bonding by the solute. The same re- t was obtained for more accurate data[58] of homologous ies with octanol-water and hexadecane-water solvent rs and predicted from a lattice-model theory.[58]

Henrian activity coefficients of a solute in both solvents hence P, may be calculated by the UNIFAC (UNI- AC Functional Group Activity Coefficients) group con- ution model[74,75,265]; the presence of co-solvent is easily resented in the calculation.

The additive-constitutive nature of log P is a property en displayed by many physico-chemical quantities. This ect has been successfully exploited[2,8] in the invention of two fragment constant additivity schemes for log P. The two methods, while similar, are not identical and differ somewhat in accuracy, applicability and ease of use.[97] Hansch and Leo's method[2] has been packaged as an interactive computer program (CLOGP).[76] In a somewhat more elaborate version (MOLY),[77] the user draws the molecular structure on a graphics terminal.

2.2.b. Other correlations

Both Hansch and Leo's[2] and Rekker's[8] fragment additivity schemes tend to be inaccurate for compounds with multiple halogen substitution. A nonlinear function has been devised[78] for multiply-substituted aromatic and heterocyclic compounds. A number of other quantities with which log P has been correlated are listed here:

-solute retention indices on two stationary phases in gas chromatography[67] (useful for volatile solutes)
-solute molar volume[58]
-solute molecular surface area[79-81]
-charge density[40,82]
-solvatochromic parameters[83,99]
- molar refraction[84]
- solvent-dependent conformational analysis (SCAP)[85]
-parachor[86,87]
- membrane cell potentials[88]
-elution times for adsorption on Tygon tubing[89]
-molecular connectivity[90]

3. Comparison of Methods of Measurement or Estimation

When one or more log P values of a substance are available to a user or evaluator who wishes to place an uncertainty on the single value, or deduce the most probably accurate value, the following considerations are pertinent: (i) the method of measurement or estimation used, together with any available experimental details, (ii) the perceived competence of the measuring laboratory or investigator, (iii) the date of the measurement. Knowledge of the general characteristics of methods of measurement of published P values is necessary for evaluation, even though their usefulness may be qualified by considerations (ii) and (iii) above in certain cases. Table 2 presents characteristics of some direct and indirect methods. Useful discussion is available, along with some tabulated results of intra- and inter-laboratory measurements by different methods.[11,67,91–94] The consequences of the various considerations in Table 2 are discussed in Sec. 5 below.

4. Retrieval of Data

The basis of the literature search was the Pomona College log P Database, created and maintained by Prof. Hansch and Leo. It is the most complete compilation of its kind, available online (Technical Database Services, Inc., 10 Columbus Circle, New York, NY 10019) and updated twice yearly. The version of July 1987 was used for the present work. For January 1987–June 1988 the Subject Index of Chemical Abstracts was used to ensure a more complete

TABLE 2. General characteristics of some measurement and estimation methods for P.

Method	Optimal log P range (approx.)	Applicability	Strengths	Weaknesses
Shake-flask (SF)	– 2.5 to 4.5	General neutral species	Direct method Reliable when precautions taken	Time-consuming Requires attention t many details of procedure Less accurate at log $P > 5$ Temperature control be inefficient
Generator column (G)	2 to 7	General, except for very hydrophilic compounds	Direct method No danger of emulsion Closed system Efficient temperature control Faster than SF	Column becomes strip of solute New column needed each solute Limited to lipophili compounds Rather elaborate analytical equipmer
Reverse-phase high-pressure liquid chromatography (HPLC)	0 to 6	Neutral species only	Fast, convenient Impurities do not interfere Analysis not required	Correlational methc Single correlation pl not accurate
Water solubility correlation	2 to 6	Neutral species of limited water solubility	Convenient Has thermodynamic basis	Correlational methc Single correlation pl inaccurate
Henrian activity coefficients	Depends upon route to activity coefficient	Neutral species	Thermodynamically exact	Ease of measurement accuracy depends up route to activity coefficient
Fragmental constants	Same as SF, useful for extrapolation	Same as SF	Fast, convenient Reliable for molecules with not many polar groups	Requires expertise f complicated molecul Usable only for functi groups covered in sche

coverage. During consultation of original articles, a number of other useful references were found and were incorporated into the present compilation.

For every log P datum of compounds investigated, the original literature reference was consulted, whenever available; in the case of direct methods of measurement, the following information was retrieved (its importance has been pointed out recently[98]):

- -temperature of measurement
- -equilibration method
- -analytical method
- -aqueous phase (water, buffer, etc.)
- -which phase(s) was analyzed
- -if no details were given but a reference was made to another publication, this was noted and the information retrieved.

It was decided to include also a number of log P values obtained by indirect methods, since these are useful for evaluation and, at times, are the only reports available.

Of course, the original articles did not always contain any or all the information sought, but whatever was available was retrieved. The source of a number of the data in the Pomona College Database are unpublished results from, or private communications to Dr. Hansch and Dr. Leo. No experimental details are available concerning these data; in the present evaluation they are classed as direct mea ments. No log P values calculated from fragment cons appear in the compilation, although estimates by Hansch and Leo and Rekker methods were used occasi ly as aids in evaluation. In the case of ionizable compo the log P value given by the author or in the Datab whether corrected for ionization or not—was recorde data were corrected by the present evaluator.

5. Criteria for Evaluation

The evaluator wishes to have as many aids and to can be found; the number and power of these tools va cording to the subject in hand. For example, in the cr evaluation of binary phase diagrams,[95] available excess modynamic data and other thermodynamic const (Gibbs–Duhem equation, phase rule, etc.) provide rel ly stringent and objective guidelines to data evaluatio the case of P, however, most of these constraints ar applicable, and the thermodynamics of solute distribut inadequate at present to provide such constraints.[21] Onl Gibbs energy of distribution is well summarized in the tive fragment constant schemes; the corresponding entl of distribution data are, however, absent for the most

Wherever both direct and indirect methods are repre- ted in the log P values for a given compound, more ight is given to those from direct methods. When neces- y or possible, directly determined values are further ighted by the availability of experimental details. In the mona College Data Base—and also in the present compi- on—Hansch and Leo's selected values are indicated by asterisk. This is a valuable guide in evaluation. In some es, a recently determined (or redetermined) value by di- t method under optimum conditions is a deciding factor. doubtful cases where the spread in reported values is wide, no direct determinations are at hand, it is helpful to con- er simultaneously the value from fragment constant emes. The Hansch and Leo method was followed in a ghtly simplified version,[96] and the Rekker method also in a plified version.[92] It has been found[97] that both methods erally yield similar results, particularly for the simple lecules considered in the present work.

In those cases where only an asterisked log P value is orted, an uncertainty of 10%—considered a fair esti- te[92]—was assigned. Where the recommended value fers markedly from experimental values, this was because re weight was given to log P from additivity schemes; the certainty is correspondingly larger.

Based on these considerations, a recommended value is en for each compound, together with an uncertainty ±) in parentheses. This uncertainty is neither simply the ndard deviation of all recorded values nor does it repre- t the total range of all recorded values. Rather it repre- ts the range in which, in the evaluator's judgment, the e value lies. Thus the uncertainty may be large when only e reported datum exists, and smaller according to the mber and consistency of reported data. It should be clear m the discussion to this point that there is always an irre- cible minimum of arbitrariness in this kind of evaluation.

6. Presentation of Data in Tables 3–20

Retrieved data for 600 simple organic compounds are sented in these Tables according to chemical type:

Table No.	Class of compound
3	Alkanes
4	Alkenes and alkynes
5	Aromatics
6	Cycloalkanes and cycloalkenes
7	Mixed-type hydrocarbons
8	Ethers
9	Alcohols
10	Aldehydes
11	Ketones
12	Acids
13	Esters
14	Halogenated compounds
15	Amines
16	Nitriles
17	Nitro compounds
18	Amides
19	Sulphur compounds
20	Other

thin each table, the general order is by increasing carbon mber, then by increasing number of hydrogen atoms. mers are listed in increasing degree of branching, and in the order of primary, secondary, and tertiary compounds. The only exception to these rules is in Table 13 (Esters) where the esters are listed according to the parent acid, e.g.,

Formic acid, *n*-propyl ester
Formic acid, phenyl ester
Acetic acid, methyl ester
Acetic acid, ethyl ester
etc.

but the other rules are adhered to.

Each compound is identified by, from left to right, the chemical formula, name(s) and CAS Registry number. The order of elements in the chemical formula is C,H,N,O,(Br,Cl,F,I),S. For acids and amines only, these are followed by the acid dissociation constant, pK_a. Unless otherwise noted, these are for 25 °C and were taken from standard references[100–103] or from original articles. Some were estimated from data for similar compounds or according to well established methods[96].

The retrieved data themselves, for each compound, are presented under nine column headings. From left to right these are:

log P-the datum quoted in the study under consideration
Asterisk (*): Hansch and Leo selected value,
?: Doubtful value;

Code-this identifies the type of method used for determination:
D: direct method,
I: indirect method,
?: information insufficient or unavailable;

Ref.-source of data. Personal communications to, or unpublished data in the Pomona College Data Base are all assigned to Ref. 104.

Temp.-where original report mentioned temperature, this is indicated (in °C).
AMB: temperature quoted as "ambient;"

Equil. Method-method of equilibration:
GC: generator column
SF: shake-flask;

Anal. method-method used for analysis of the phases:
AS: absorption spectrophotometry,
CR: chemical reaction,
FL: fluorescence,
GLC: gas-liquid chromatography,
HPLC: high-pressure liquid chromatography,
K: Kjeldahl analysis for *N*,
RC: Radiochemical,
TN: acid–base titration;

Aq. phase-nature of the aqueous phase:
W: octanol-saturated water,
NS: neutral salt solution,
pHxxx: buffer solution of stated pH;

Phase(s) analyzed-AQ: aqueous,
ORG: organic,
one: either aqueous or organic (not specified);

Method ref.-investigator's stated source for method.

The indirect methods used to determine log P values are indicated by short phrases (water solubility correlation, HPLC, etc.). The D and I values are listed in separate groups and placed in increasing order within each group. The last entry for each compound is a recommended log P value, with uncertainty in parentheses.

Auxiliary information is provided in footnotes a end of each table. In Tables 12 and 15, ion corrected values (reported at source) are footnoted as such. All o are not ion corrected.

Table 3. Alkanes

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_5H_{12}	n-Pentane	CAS # 109-66-0						
2.50	D	30		SF	GLC	W	AQ	46
2.50	D	105		SF				
3.23	D	104	0				Both	
*3.39	D	104					Both	
3.62	D	9,10	25	G	GLC	W	Both	11
3.62	D	58	25	G	GLC	W	Both	9
3.60	I	58	25	from measured activity coefficients				
3.64	I	10		from measured activity coefficients				
3.45 (0.20) Recommended								
C_5H_{12}	2,2-Dimethylpropane (neopentane)	CAS # 463-82-1						
*3.11	D	104						
3.11 (0.20) Recommended								
C_6H_{14}	n-Hexane	CAS # 110-54-3						
4.11	D	9,10	25	G	GLC	W	Both	11
4.11	D	58	25	G	GLC	W	Both	11
3.00?	I	42		head-space chromatographic method				107
3.90	I	106	20	from measured activity coefficients				
4.16	I	58	25	from measured activity coefficients				
4.20	I	10	25	from measured activity coefficients				
4.25	I	22	25	from measured activity coefficients				
4.00 (0.25) Recommended								
C_6H_{14}	3-Methylpentane	CAS # 96-14-0						
2.80?	I			head-space chromatographic method				107
3.60 (0.20) Recommended								
C_6H_{14}	2,2-Dimethylbutane	CAS # 75-83-2						
*3.82	D	104					Both	
3.82 (0.40) Recommended								
C_6H_{14}	2,3-Dimethylbutane	CAS # 79-29-8						
*3.85	D	104					Both	
3.85 (0.40) Recommended								

Table 3. Alkanes (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_6H_{14}	2,3-Dimethylbutane CAS # 79-29-8							
*3.85	D	104					Both	
3.85 (0.40) Recommended								
C_7H_{14}	n-Heptane CAS # 142-82-5							
4.66	D	9,10	25	G	GLC	W	Both	11
4.66	D	58	25	G	GLC	W	Both	9
4.48	I	22	25	from measured activity coefficients				
4.73	I	58	25	from measured activity coefficients				
4.76	I	10	25	from measured activity coefficients				
4.50 (0.25) Recommended								
C_8H_{18}	n-Octane CAS # 111-65-9							
5.18	D	9,10	25	G	GLC	W	Both	11
5.18	D	58	25	G	GLC	W	Both	9
4.00?	I	109		head-space chromatographic method				42,107
5.24	I	58	25	from measured activity coefficients				
5.29	I	10	25	from measured activity coefficients				
5.15 (0.45) Recommended								
C_9H_{20}	n-Nonane CAS # 111-84-2							
4.51	I	109		head-space chromatographic method				42,107
5.65 (0.60) Recommended								
$C_{10}H_{22}$	n-Decane CAS # 124-18-5							
5.01	I	109		head-space chromatographic method				42,107
6.25 (0.70) Recommended								
$C_{12}H_{26}$	n-Dodecane CAS # 112-40-3							
5.64[a]	D	110						
6.10	I	109		head-space chromatographic method				42,107
6.80 (1.00) Recommended								
$C_{14}H_{30}$	n-Tetradecane CAS # 629-59-4							
7.20	I	109		head-space chromatographic method				42,107
8.00 (1.00) Recommended								

[a] W. E. Hammers, personal communication

Table 4. Alkenes and alkynes

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_4H_6	1,3-Butadiene		CAS # 106-99-0					
*1.99	D	104					Both	
1.99	(0.20) Recommended							
C_4H_6	2-Butyne		CAS # 503-17-3					
*1.46	D	104					Both	
1.46	(0.20) Recommended							
C_4H_8	cis-2-Butene		CAS # 590-18-1					
*2.33	D	104					Both	
2.33	(0.30) Recommended							
C_4H_8	trans-2-Butene		CAS # 624-64-6					
*2.31	D	104					Both	
2.31	(0.30) Recommended							
C_4H_8	2-Methylpropene (isobutene)		CAS # 115-11-7					
*2.34	D	104					Both	
*2.40	D	104					Both	
2.35	(0.40) Recommended							
C_5H_8	1,4-Pentadiene		CAS # 591-93-5					
*2.48	D	104					Both	
2.48	(0.30) Recommended							
C_5H_8	1-Pentyne		CAS # 627-19-0					
*1.98	D	30,111	25	SF	GLC	W	One	46
2.12	D	9,10	25	G	GLC	W	Both	11
1.98	(0.20) Recommended							
C_6H_{10}	1,5-Hexadiene		CAS # 592-42-7					
2.45?	D	104						
2.80	(0.30) Recommended							

Table 4. Alkenes and alkynes (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_6H_{10}	1-Hexyne		CAS # 693-02-7					
2.73	D	9,10	25	G	GLC	W	Both	11
2.73	(0.30) Recommended							
C_6H_{12}	1-Hexene		CAS # 592-41-6					
*3.39	D	9	25	G	GLC	W	Both	11
3.39	D	58	25	G	GLC	W	Both	9
3.47	D	10	25	G	HPLC	W	Both	
3.40	I	58	25	from measured activity coefficients				
3.47	I	10	25	from measured activity coefficients				
3.40	(0.10) Recommended							
C_7H_{14}	1-Heptene		CAS # 592-76-7					
*3.99	D	9,10	25	G	GLC	W	Both	11
3.99	D	58	25	G	GLC	W	Both	9
4.06	I	58	25	from measured activity coefficients				
3.99	(0.10) Recommended							
C_8H_{16}	1-Octene		CAS # 111-66-0					
4.56	D	58	25	G	GLC	W	Both	9
*4.57	D	9	25	G	GLC	W	Both	11
4.88	D	10	25	G	HPLC	W	Both	
4.72	I	58	25	from measured activity coefficients				
4.76	I	10	25	from measured activity coefficients				
4.57	(0.20) Recommended							
C_9H_{18}	1-Nonene		CAS # 124-11-8					
*5.15	D	9	25	G	GLC	W	Both	11
5.15	D	58	25	G	GLC	W	Both	9
5.35	D	10	25	G	HPLC	W	Both	
5.31	I	58	25	from measured activity coefficients				
5.34	I	10	25	from measured activity coefficients				
5.15	(0.20) Recommended							

Table 5. Aromatics

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_6H_6	Benzene		CAS # 71-43-2					
1.56	D	40	25	SF	AS	pH7.4	Both	117
2.01	D	58	25	G	HPLC	W	Both	11
2.03	D	104				a	Both	
2.04	D	104				D_2O	Both	
2.04	D	115		SF	AS	NS	AQ	
2.11	D	113	25	SF	AS	W	Both	
2.12	D	108	23	SF	RC	W	Both	
*2.13	D	46	25	SF	AS	W	AQ	
2.13	D	114	25	SF	GLC	W	AQ	
2.13	D	10	25	G	HPLC	W		
2.15	D	104						
2.15	D	104					Both	
2.19	D	104				pH2.7		
1.83^c	I	65		HPLC				
1.90	I	33		from water solubility correlation				
1.98	I	58		from measured activity coefficients				
2.03	I	10	25	from measured activity coefficients				
2.13	I	106	25	from measured activity coefficients				28,29
2.15	I	74	25	from UNIFAC activity coefficients				
2.17^b	I	64		HPLC				
2.31	I	116		HPLC				
2.34	I	112		HPLC				
2.13 (0.10) Recommended								
C_6D_6	Hexadeuterobenzene			CAS # 1076-43-3				
2.03	D	115		SF	AS	NS	AQ	
2.03 (0.20) Recommended								
C_7H_8	Toluene		CAS # 108-88-3					
2.11	D	40	25	SF	AS	pH7.4	Both	117
2.21	D	108	23	SF	RC	W	Both	
2.61	D	115		SF	AS	NS	AQ	
2.65	D	9,10	25	G	HPLC	W	Both	11
2.65	D	58	25	G	HPLC	W	Both	11
2.68	D	118	23	SF	HPLC	W	Both	
2.69	D	46	25	SF	AS	W	AQ	
*2.73	D	104						
2.80	D	104						

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_8	Toluene (continued)							
2.51	I	33	25	from water solubility correlation				
2.51^c	I	65		HPLC				
2.64	I	58	25	from measured activity coefficients				
2.65	I	64		HPLC				
2.66	I	10	25	from measured activity coefficients				
2.76	I	74	25	from UNIFAC activity coefficients				
2.77	I	119		HPLC				
2.88	I	75	25	from UNIFAC activity coefficients				
2.94	I	112		HPLC				
2.73	(0.10)	Recommended						
C_7D_8	Octadeuterotoluene			CAS # 2037-26-5				
2.57	D	115		SF	AS	NS	AQ	
2.57	(0.20)	Recommended						
C_8H_{10}	1,2-Dimethylbenzene (o-xylene)			CAS # 95-47-6				
*3.12	D	104						
3.13	D	9,10	25	G	HPLC	W	Both	11
2.77	D	104						
3.04	I	33	25	from water solubility correlation				
3.04^c	I	65		HPLC				
3.15	I	10	25	from measured activity coefficients				
3.12	(0.20)	Recommended						
C_8H_{10}	1,3-Dimethylbenzene (m-xylene)			CAS # 108-38-3				
*3.20	D	104						
3.20	D	9,10	25	G	HPLC	W	Both	11
3.22^c	I	65		HPLC				
3.25	I	10	25	from measured activity coefficients				
3.37	I	57		HPLC				
3.20	(0.20)	Recommended						
C_8H_{10}	1,4-Dimethylbenzene (p-xylene)			CAS # 106-42-3				
*3.15	D	104						
3.18	D	9,10	25	G	HPLC,GLC	W	Both	11
3.08	I	42		head-space chromatographic method				107
3.15^c	I	65		HPLC				
3.52	I	75	25	from UNIFAC activity coefficients				
3.15	(0.20)	Recommended						

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_8H_{10}	Ethylbenzene		CAS # 100-41-1					
3.13	D	9,10	25	G	HPLC	W	Both	11
3.13	D	58	25	G	HPLC	W	Both	11
*3.15	D	120		SF	AS	W	AQ	46
3.07[c]	I	65		HPLC				
3.10	I	33	25	from water solubility correlation				
3.12	I	122		HPLC				
3.14	I	58	25	from measured activity coefficients				
3.15	I	10	25	from measured activity coefficients				
3.28	I	75	25	from UNIFAC activity coefficients				
3.15 (0.20) Recommended								
C_9H_8	Indene		CAS # 95-13-6					
*2.92	D	104						
3.26	I	65		HPLC				
2.92 (0.20) Recommended								
C_9H_{12}	n-Propylbenzene		CAS # 103-65-1					
3.44	D	118	23	SF	HPLC	W	Both	
3.57	D	104						
3.68	D	120		SF	AS	W	AQ	46
3.69[d]	D	9,10	25	G	HPLC	W	Both	
3.69	D	58	25	G	HPLC	W	Both	11
*3.72[b]	D	11	25	SF,G	HPLC	W	Both	
3.59	I	33	25	from water solubility correlation				
3.60	I	42		head-space chromatographic method				107
3.69	I	121		HPLC				
3.71	I	58	25	from measured activity coefficients				
3.73	I	10	25	from measured activity coefficients				
3.90	I	121		HPLC				
3.69 (0.15) Recommended								
C_9H_{12}	Isopropylbenzene		CAS # 98-82-8					
*3.66	D	104						
3.66	D	104						
3.51	I	42		head-space chromatographic method				107
3.52	I	122		HPLC				
3.63	I	33	25	from water solubility correlation				
3.66 (0.20) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_9H_{12}	1,2,3-Trimethylbenzene			CAS # 526-73-8				
3.55	D	9,10	25	G	HPLC	W	Both	11
*3.66	I	121		HPLC				
3.60	(0.20)	Recommended						
C_9H_{12}	1,2,4-Trimethylbenzene			CAS # 95-63-6				
3.63	D	10	25	G	HPLC	W	Both	
3.58	I	33	25	from water solubility correlation				
*3.78	I			HPLC				
3.63	(0.15)	Recommended						
C_9H_{12}	1,3,5-Trimethylbenzene (mesitylene)				CAS # 108-67-8			
*3.42	D	104						
3.84	I	121		HPLC				
4.15	I	75	25	from UNIFAC activity coefficients				
3.42	(0.30)	Recommended						
C_9H_{12}	1-Methyl-2-ethylbenzene (2-ethyltoluene)				CAS # 611-14-3			
*3.53	D	9,10	25	G	HPLC	W	Both	11
3.63	I	42		head-space chromatographic method				107
3.53	(0.30)	Recommended						
C_9H_{12}	1-Methyl-4-ethylbenzene (4-ethyltoluene)				CAS # 622-96-8			
3.63	I	42		head-space chromatographic method				107
3.63	(0.40)	Recommended						
$C_{10}H_8$	Naphthalene		CAS # 91-20-3					
3.01	D	40	25	SF	AS	pH7.4	Both	117
3.28	D	94		SF		W	AQ	
*3.30	D	104						
3.35	D	68		SF	GLC	W	Both	
3.35	D	10	25	G	HPLC	W	Both	
3.36	D	86	20	SF	GLC	W	AQ	46
3.36	D	113	25	SF	AS	W	Both	
3.37	D	124						
3.40	D	126	23	SF	FL	W	AQ	

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_8$	Naphthalene (continued)							
3.45	D	125		SF				1
3.59	D	104						
3.17	I	56		HPLC				
3.29	I	119		HPLC				
3.30	I	33	25	from water solubility correlation				
3.30[b]	I	64		HPLC				
3.35	I	42		head-space chromatographic method				107
3.43	I	65		HPLC				
3.65	I	75	25	from UNIFAC activity coefficients				
3.35 (0.10) Recommended								
$C_{10}H_8$	Azulene	CAS # 275-51-4						
*3.20	D	104						
3.22	D	127		SF	AS	W	ORG	3
3.22 (0.20) Recommended								
$C_{10}H_{14}$	n-Butylbenzene	CAS # 104-51-8						
*4.26	D	104						
4.28	D	9,10	25	G	HPLC,GLC	W	Both	11
4.29	D	58	25	G	HPLC	W	Both	11
4.01	I	42		head-space chromatographic method				107
4.18	I	68	25	from water solubility correlation				
4.34	I	58	25	from measured activity coefficients				
4.44	I	121		HPLC				
4.26 (0.15) Recommended								
$C_{10}H_{14}$	tert-Butylbenzene	CAS # 98-06-6						
4.07	D	118	23	SF	HPLC	W	Both	
*4.11	D	104						
4.11	D	104						
4.11 (0.10) Recommended								
$C_{10}H_{14}$	1-Methyl-4-isopropylbenzene (p-cymene)	CAS # 25155-15-1						
*4.10	D	108	23	SF	RC	W	Both	
4.14	I	74	25	from UNIFAC activity coefficients				
4.10 (0.10) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_{14}$	1,2,3,4-Tetramethylbenzene			CAS # 488-23-3				
3.98	D	10	25	G	HPLC	W	Both	
*4.11	I	121		HPLC				
4.00 (0.20) Recommended								
$C_{10}H_{14}$	1,2,3,5-Tetramethylbenzene			CAS # 527-53-7				
4.04	D	10	25	G	HPLC	W	Both	
*4.17	I	121		HPLC				
4.10 (0.20) Recommended								
$C_{10}H_{14}$	1,2,4,5-Tetramethylbenzene			CAS # 95-93-2				
*4.00	D	104						
2.80?	I	42		head-space chromatographic method				107
4.24	I	123		HPLC				
4.10 (0.20) Recommended								
$C_{11}H_{10}$	1-Methylnaphthalene			CAS # 90-12-0				
*3.87	D	126	23	SF	FL	W	AQ	
3.95	I	33	25	from water solubility correlation				
3.87 (0.20) Recommended								
$C_{11}H_{10}$	2-Methylnaphthalene			CAS # 91-57-6				
*3.86	D	126	23	SF	FL	W	AQ	
4.11	D	113	25	SF	AS	W	Both	
3.90	I	33	25	from water solubility correlation				
4.01	I	65		HPLC				
4.09	I	119		HPLC				
4.00 (0.20) Recommended								
$C_{11}H_{16}$	n-Pentylbenzene			CAS # 538-68-1				
4.90	D	9,10	25	G	HPLC	W	Both	11
4.90 (0.30) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{11}H_{16}$	Pentamethylbenzene			CAS # 700-12-9				
*4.56	I	121		HPLC				
4.57	I	123		HPLC				
4.56 (0.40) Recommended								
$C_{12}H_{10}$	Biphenyl	CAS # 92-52-4						
3.16	D	40	25	SF	AS	pH7.4	Both	117
3.76	D	34	25	G	GLC	W	Both	11
3.89	D	129	25	G	HPLC	W	Both	
3.91	D	92		SF				
3.95	D	104						
4.04	D	125		SF				1
4.04	D	108	23	SF	HPLC	W	Both	
3.63	I	130		HPLC				
3.70^{b}	I	64		HPLC				
3.75	I	56		HPLC				
3.77	I	116		HPLC				
3.79	I	128		HPLC				
4.01	I	65		HPLC				
4.02	I	42		head-space chromatographic method				107
4.06	?	131						
4.10	I	68	25	from water solubility correlation				
4.13	I	119		HPLC				
4.14	I	33	25	from water solubility correlation				
4.24	I	37		from solubility ratio				
4.25	I	74	25	from UNIFAC activity coefficients				
3.98 (0.10) Recommended								
$C_{12}H_{10}$	Acenaphthene		CAS # 83-32-9					
3.91^{b,e}	D	110		SF				
*3.92	D	108	23	SF	RC	W	Both	
4.15	I	33	25	from water solubility correlation				
4.43	I	74	25	from UNIFAC activity coefficients				
3.92 (0.25) Recommended								
$C_{12}H_{12}$	1-Ethylnaphthalene			CAS # 1127-76-0				
*4.39	D	38	23	SF	FL	W	AQ	
4.42	I	33	25	from water solubility correlation				
4.40 (0.40) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{12}H_{12}$	2-Ethylnaphthalene			CAS # 939-27-5				
*4.38	D	126	23	SF	FL	W	AQ	
4.38 (0.50) Recommended								
$C_{12}H_{12}$	1,2-Dimethylnaphthalene			CAS # 573-98-8				
*4.31	D	126	23	SF	FL	W	AQ	
4.31 (0.40) Recommended								
$C_{12}H_{12}$	1,3-Dimethylnaphthalene			CAS # 575-41-7				
*4.42	D	126	23	SF	FL	W	AQ	
4.55	I	33	25	from water solubility correlation				
4.42 (0.30) Recommended								
$C_{12}H_{12}$	1,4-Dimethylnaphthalene			CAS # 571-58-4				
*4.37	D	126	23	SF	FL	W	AQ	
4.39	I	33	25	from water solubility correlation				
4.37 (0.30) Recommended								
$C_{12}H_{12}$	1,5-Dimethylnaphthalene			CAS # 571-61-9				
*4.38	D	126	23	SF	FL	W	AQ	
4.35	I	33	25	from water solubility correlation				
4.38 (0.30) Recommended								
$C_{12}H_{12}$	1,7-Dimethylnaphthalene			CAS # 575-37-1				
*4.44	D	126	23	SF	FL	W	AQ	
4.44 (0.30) Recommended								
$C_{12}H_{12}$	1,8-Dimethylnaphthalene			CAS # 569-41-5				
*4.26	D	126	23	SF	FL	W	AQ	
4.26 (0.30) Recommended								
$C_{12}H_{12}$	2,6-Dimethylnaphthalene			CAS # 581-42-0				
*4.31	D	126	23	SF	FL	W	AQ	
4.32	I	33	25	from water solubility correlation				
4.31 (0.30) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{12}H_{18}$	n-Hexylbenzene		CAS # 1077-16-3					
*5.52	D	9,10	25	G	HPLC	W	Both	11
5.24	I	68	25	from water solubility correlation				
5.52 (0.30) Recommended								
$C_{12}H_{18}$	Hexamethylbenzene			CAS # 87-85-4				
4.31	D	104						
4.61	D	10	25	G	HPLC	W	Both	
5.00	I	123		HPLC				
*5.11	I	121		HPLC				
4.75 (0.25) Recommended								
$C_{13}H_{10}$	Fluorene		CAS # 86-73-7					
*4.18	D	104						
4.18	D	132		SF	GLC	pH7	Both	
4.18	D	37	30	SF	AS	W	Both	
4.18	I	68	25	from water solubility correlation				
4.23	I	119		HPLC				
4.27	I	33	25	from water solubility correlation				
4.34	I	37	25	from solubility ratio				
4.18 (0.20) Recommended								
$C_{13}H_{12}$	Diphenylmethane			CAS # 101-81-5				
*4.14	D	104						
4.22	I	65		HPLC				
4.14 (0.20) Recommended								
$C_{13}H_{12}$	4-Methylbiphenyl			CAS # 644-08-6				
4.63	D	81	25	G	GLC	W	Both	129
4.66	I	119		HPLC				
4.63 (0.20) Recommended								
$C_{13}H_{14}$	1,4,5-Trimethylnaphthalene				CAS # 2131-41-1			
4.79	I	33	25	from water solubility correlation				
5.10 (0.50) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{13}H_{14}$ 2,3,6-Trimethylnaphthalene CAS # 829-26-5								
*4.73	D	126	23	SF	FL	W	AQ	
4.73 (0.40) Recommended								
$C_{14}H_{10}$ Anthracene CAS # 120-12-7								
*4.45	D	124		SF				
4.45	D	132		SF	GLC	pH7	Both	
4.54	D	113	25	SF	AS	W	Both	
3.45?	I	56		HPLC				
4.20	I	122		HPLC				
4.51	I	65		HPLC				
4.60	I	64		HPLC				
4.63	I	42		head-space chromatographic method				107
4.63	I	119		HPLC				
4.73	I	33	25	from water solubility correlation				
4.80	I	130		HPLC				
4.50 (0.15) Recommended								
$C_{14}H_{10}$ Phenanthrene CAS # 85-01-8								
*4.46	D	124		SF				
4.52	D	92		SF				
4.57	D	113	25	SF	AS	W	Both	
4.28	I	57		HPLC				
4.31	I	92		HPLC				
4.50	I	119		HPLC				
4.63	I	42		head-space chromatographic method				107
4.64	I	33	25	from water solubility correlation				
4.52 (0.15) Recommended								
$C_{14}H_{12}$ trans-1,2-Diphenylethene (trans-stilbene) CAS # 103-30-0								
*4.81	D	104						
4.81 (0.40) Recommended								
$C_{14}H_{12}$ 1-Methylfluorene CAS # 1730-37-6								
*4.97[f]	D	38						
4.97	I	119		HPLC				
4.97 (0.30) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{14}H_{12}$ 9,10-Dihydroanthracene CAS # 613-31-0								
*4.25	D	104						
4.25 (0.30) Recommended								
$C_{14}H_{14}$ Bibenzyl (1,2-diphenylethane) CAS # 103-29-7								
*4.79	D	104						
4.82	D	104						
4.60	I	116		HPLC				
4.71	I	65		HPLC				
4.82	I	37		from solubility ratio				
4.70 (0.20) Recommended								
$C_{14}H_{14}$ 4,4'-Dimethylbiphenyl CAS # 613-33-2								
5.09	D	81	25	G	GLC	W	Both	129
5.09 (0.30) Recommended								
$C_{14}H_{22}$ 1-Phenyloctane (n-octylbenzene) CAS # 2189-60-8								
6.30	D	68		SF	GLC	W	Both	
6.30 (0.40) Recommended								
$C_{15}H_{12}$ 1-Methylphenanthrene CAS # 832-69-9								
5.08	I	119		HPLC				
5.08 (0.40) Recommended								
$C_{15}H_{12}$ 2-Methylphenanthrene CAS # 2531-84-2								
5.24	I	119		HPLC				
5.24 (0.40) Recommended								
$C_{15}H_{12}$ 3-Methylphenanthrene CAS # 832-71-3								
5.15	I	119		HPLC				
5.15 (0.40) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{15}H_{12}$	9-Methylanthracene			CAS # 779-02-2				
*5.07	D	113	25	SF	AS	W	Both	
4.96	I	99		from solvatochromic parameters				
5.07	I	38	25	from water solubility correlation				
5.10	I	119		HPLC				
5.65	I	33	25	from water solubility correlation				
5.07 (0.20) Recommended								
$C_{16}H_{10}$	Pyrene		CAS # 129-00-0					
*4.88	D	104						
5.09	D	133	AMB	SF	RC	W	Both	134,135
5.18	D	113	25	SF	AS	W	Both	
4.50	I	122		HPLC				
5.08	I	119		HPLC				
5.12	I	33	25	from water solubility correlation				
5.22	I	42		head-space chromatographic method				107
5.00 (0.20) Recommended								
$C_{16}H_{10}$	Fluoranthene		CAS # 206-44-0					
5.20^g	D	136						
4.85	I	119		HPLC				
5.22	I	38	25	from water solubility correlation				
5.29	I	33	25	from water solubility correlation				
5.20 (0.20) Recommended								
$C_{16}H_{14}$	2-Ethylanthracene			CAS # 52251-71-5				
5.85	I	119		HPLC				
5.85 (0.30) Recommended								
$C_{16}H_{14}$	9,10-Dimethylanthracene			CAS # 781-43-1				
5.25	I	38	25	from water solubility correlation				
5.25	I	33	25	from water solubility correlation				
5.48	I	99		from solvatochromic parameters				
5.69	I	119		HPLC				
5.69 (0.40) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{16}H_{26}$	1-Phenyldecane (n-decylbenzene)			CAS # 104-72-3				
7.35	D	68		SF	GLC	W	Both	
7.35 (0.40) Recommended								
$C_{17}H_{12}$	1,2-Benzofluorene (benz(a)fluorene)			CAS # 238-84-6				
5.32	I	38	25	from water solubility correlation				
5.32	I	33	25	from water solubility correlation				
5.68	I	119		HPLC				
5.40 (0.40) Recommended								
$C_{17}H_{12}$	2,3-Benzofluorene (benz(b)fluorene)			CAS # 243-17-4				
5.75	I	38	25	from water solubility correlation				
5.77	I	119		HPLC				
5.75 (0.40) Recommended								
$C_{18}H_{12}$	9,10-Benzophenanthrene (triphenylene)			CAS # 217-59-4				
5.49	I	119		HPLC				
5.49 (0.50) Recommended								
$C_{18}H_{12}$	1,2-Benzanthracene (benz(a)anthracene)			CAS # 56-55-3				
5.91	I	38	25	from water solubility correlation				
6.10	I	33	25	from water solubility correlation				
5.79	I	119		HPLC				
5.91 (0.40) Recommended								
$C_{18}H_{12}$	Naphthacene (benz(b)anthracene)			CAS # 92-24-0				
*5.90	D	113	25	SF	AS	W	Both	
5.48	I	99		from solvatochromic parameters				
5.54	I	33	25	from water solubility correlation				
5.76	I	119		HPLC				
5.90	I	38	25	from water solubility correlation				
5.76 (0.30) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{18}H_{12}$	Chrysene		CAS # 218-01-9					
5.91	D	68		SF	GLC	W	Both	
5.73	I	119		HPLC				
5.79	I	38	25	from water solubility correlation				
6.01	I	33	25	from water solubility correlation				
5.86 (0.40) Recommended								
$C_{18}H_{14}$	4-Phenylbiphenyl (p-terphenyl)		CAS # 26140-60-3					
*6.03	I	123		HPLC				
6.03 (0.50) Recommended								
$C_{20}H_{12}$	Perylene		CAS # 198-55-0					
5.82	I	119		HPLC				
6.50	I	38	25	from water solubility correlation				
6.53	I	33	25	from water solubility correlation				
6.25 (0.50) Recommended								
$C_{20}H_{12}$	3,4-Benzopyrene (benz(a)pyrene)		CAS # 50-32-8					
6.00	D	137	23	SF	AS	W	Both	
6.50	D	68		SF	GLC	W	Both	
*5.97	I	137		HPLC				
5.98^{f}	I	38	25	from water solubility correlation				
6.04	I	119		HPLC				
6.50	I	128		HPLC				
6.57	I	33	25	from water solubility correlation				
6.78	I	6		HPLC				
6.83	I	138		HPLC				
6.35 (0.40) Recommended								
$C_{20}H_{12}$	3,4-Benzofluoranthene		CAS # 205-99-2					
5.78	I	119		HPLC				
5.78 (0.50) Recommended								
$C_{20}H_{14}$	9-Phenylanthracene		CAS # 602-55-1					
6.01	I	119		HPLC				
6.01 (0.50) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{20}H_{16}$	7,12-Dimethylbenz(a)anthracene				CAS # 57-97-6			
*5.80	D	133	AMB	SF	RC	W	Both	134
5.80 (0.50) Recommended								
$C_{21}H_{16}$	3-Methylcholanthrene			CAS # 56-49-5				
*6.42	D	133	AMB	SF	RC	W	Both	134
6.69	I	33	25	from water solubility correlation				
7.11	I	38	25	from water solubility correlation				
6.75 (0.50) Recommended								
$C_{22}H_{12}$	Benzo(g,h,i)perylene			CAS # 191-24-2				
6.25	I	99		from solvatochromic parameters				
6.63	I	119		HPLC				
6.77	I	33	25	from water solubility correlation				
7.10	I	38	25	from water solubility correlation				
6.90 (0.40) Recommended								
$C_{22}H_{14}$	2,3:6,7-Dibenzanthracene (pentacene)							
7.19	I	38	25	from water solubility correlation				
7.19 (0.70) Recommended								
$C_{22}H_{14}$	1,2:3,4-Dibenzanthracene (dibenz(a,c)anthracene)							
7.19	I	38	25	from water solubility correlation				
7.19 (0.70) Recommended								
$C_{22}H_{14}$	1,2:5,6-Dibenzanthracene (dibenz(a,h)anthracene)						CAS # 53-70-3	
*6.50	D	133	AMB	SF	RC	W	Both	134
6.52	I	99		from solvatochromic parameters				
7.19	I	38	25	from water solubility correlation				
6.75 (0.40) Recommended								
$C_{22}H_{14}$	3,4-Benzonaphthacene (benz(a)naphthacene)					CAS # 226-88-0		
6.81	I	119		HPLC				
6.81 (0.70) Recommended								

Table 5. Aromatics (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{24}H_{12}$	Coronene		CAS # 191-07-1					
*5.40	I	94		HPLC				
7.64	I	38	25	from water solubility correlation				
6.5 (1.0) Recommended								

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[a] Phases were D_2O and $C_8H_{17}OD$.

[b] Average value.

[c] From a restricted correlation plot.

[d] Extrapolated to zero concentration in organic phase.

[e] D. Kotzias, personal communication

[f] It is not clear whether this is authors' value or one from the literature.

[g] W. Klopffer et al., personal communication.

Table 6. Cycloalkanes and cycloalkenes

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_5H_{10}	Cyclopentane		CAS # 287-92-3					
2.64	D	104						
*3.00	D	104						
2.05?	I	42		head-space chromatographic method				107
3.00 (0.30) Recommended								
C_6H_8	1,3-Cyclohexadiene		CAS # 592-57-4					
*2.47	D	104					Both	
2.47 (0.25) Recommended								
C_6H_8	1,4-Cyclohexadiene		CAS # 628-41-1					
*2.30	D	104						
2.30 (0.25) Recommended								
C_6H_{10}	Cyclohexene		CAS # 110-83-8					
1.90?	D	139		SF	GLC			1
*2.86	D	104					Both	
2.86 (0.25) Recommended								
C_6H_{12}	Cyclohexane		CAS # 110-82-7					
*3.44	D	104						
2.44?	I	42		head-space chromatographic method				107
3.70	I	22	25	from measured activity coefficients				
3.44 (0.35) Recommended								
C_6H_{12}	Methylcyclopentane		CAS # 96-37-7					
*3.37	D	104						
2.35?	I	42		head-space chromatographic method				107
3.37 (0.30) Recommended								
C_7H_8	1,3,5-Cycloheptatriene		CAS # 544-25-2					
*2.63	D	92		SF				
3.03	I	92		HPLC				
2.63 (0.40) Recommended								

Table 6. Cycloalkanes and cycloalkenes (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_{14}	Methylcyclohexane			CAS # 108-87-2				
2.76?	I	42		head-space chromatographic method				107
3.88 (0.40)	Recommended							
C_8H_{12}	1,5-Cyclooctadiene			CAS # 111-78-4				
3.16	D	92		SF				
3.94	I	92		HPLC				
3.55 (0.40)	Recommended							
C_8H_{16}	Cyclooctane		CAS # 292-64-8					
3.28?	I	42		head-space chromatographic method				107
4.45 (0.40)	Recommended							
$C_{10}H_{16}$	Adamantane		CAS # 281-23-2					
5.20?	D	140		SF	RC	pH7.4	Both	1
4.24 (0.50)	Recommended							
$C_{12}H_{18}$	1,5,9-Cyclododecatriene			CAS # 4904-61-4				
4.12?	D	92,142		SF				
5.65	I	141		HPLC				
5.50 (0.40)	Recommended							

Table 7. Mixed-type hydrocarbons

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_8H_6	Ethynylbenzene		CAS # 536-74-3					
*2.53	D	120		SF	AS	W	AQ	46
2.16	I	143		HPLC				
2.40 (0.25) Recommended								
C_8H_8	Phenylethene (styrene)			CAS # 100-42-5				
*2.95	D	104						
3.16	D	108	23	SF	HPLC	W	Both	
2.76	I	144		HPLC				
2.90	I	119		HPLC				
3.39	I	74	25	from UNIFAC activity coefficients				
3.05 (0.30) Recommended								
C_9H_{10}	1-Phenyl-1-propene			CAS # 637-50-3				
3.35	D	104						
3.35 (0.15) Recommended								
C_9H_{10}	3-Phenyl-1-propene (allylbenzene)				CAS # 300-57-2			
*3.23	D	104						
3.23 (0.15) Recommended								
C_9H_{10}	Indane		CAS # 496-11-7					
3.18	D	104						
3.33	D	104						
3.33 (0.30) Recommended								
C_9H_{10}	Phenylcyclopropane (cyclopropylbenzene)					CAS # 873-49-4		
*3.27	D	104						
3.27 (0.25) Recommended								
$C_{13}H_{10}$	Hept-1,3-diyn-5-enylbenzene			CAS # 13678-98-3				
4.76	I	145		HPLC				112,146
4.8 (1.0) Recommended								

Table 7. Mixed-type hydrocarbons

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{14}H_{12}$	Vinylacenaphthene (isomer not specified)							
3.99	I	119		HPLC				
3.99	(0.40)	Recommended						

Table 8. Ethers

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_2H_4O	Epoxyethane (ethylene oxide) CAS # 75-21-8							
*-0.30	D	104					Both	
-0.30	(0.20)	Recommended						
C_2H_6O	Oxapropane (dimethyl ether) CAS # 115-10-6							
*0.10	D	104					Both	
0.10	(0.20)	Recommended						
C_3H_6O	1,2-Epoxypropane (propylene oxide) CAS # 75-56-9							
*0.03	D	104						
0.03	(0.10)	Recommended						
C_4H_4O	1,4-Epoxy-1,3-butadiene (furan) CAS # 110-00-9							
*1.34	D	104					Both	
1.34	D	104						
1.13	I	123		HPLC				
1.34	(0.20)	Recommended						
C_4H_6O	1,4-Epoxy-2-butene (2,5-dihydrofuran) CAS # 1708-29-8							
*0.46	D	104					Both	
0.46	(0.25)	Recommended						

Table 8. Ethers (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_4H_8O 3-Oxa-1-pentene (ethylvinyl ether) CAS # 109-92-2								
*1.04	D	104						
1.04 (0.20) Recommended								
C_4H_8O 1,4-Epoxybutane (tetrahydrofuran) CAS # 109-99-9								
0.22	D	80		SF	GLC	W	ORG	
*0.46	D	104					Both	
0.46 (0.10) Recommended								
$C_4H_{10}O$ 3-Oxapentane (diethyl ether) CAS # 60-29-7								
0.77	D	104						
0.83	D	147	20	SF	CR	W	Both	148
*0.89	D	104					Both	
0.89 (0.10) Recommended								
C_5H_6O 2-Methylfuran CAS # 534-22-5								
*1.85	D	104						
1.85 (0.20) Recommended								
$C_5H_{10}O$ 1,5-Epoxypentane (tetrahydropyran) CAS # 142-68-7								
0.64	D	80		SF	GLC	W	ORG	
0.82 (0.20) Recommended								
$C_5H_{12}O$ 2-Oxa-3,3-dimethylbutane (methyl t-butyl ether) CAS # 1634-04-4								
*0.94	D	80		SF	GLC	W	ORG	
0.94 (0.30) Recommended								
C_6H_8O 2-Ethylfuran CAS # 3208-16-0								
*2.40	D	104						
2.40 (0.20) Recommended								
$C_6H_{10}O$ 1,2-Epoxycyclohexane CAS # 286-16-8								
1.26	D	149	37	SF	GLC	pH7.4	ORG	
1.30 (0.30) Recommended								

Table 8. Ethers (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_6H_{12}O$	cis-2,5-Dimethyltetrahydrofuran	CAS # 2144-41-4						
*1.22	D	80		SF	GLC	W	ORG	
1.22 (0.25) Recommended								
$C_6H_{12}O$	trans-2,5-Dimethyltetrahydrofuran	CAS # 2390-94-5						
*1.34	D	80		SF	GLC	W	ORG	
1.34 (0.25) Recommended								
$C_6H_{14}O$	4-Oxaheptane (di-n-propyl ether)	CAS # 111-43-3						
*2.03	D	104						
2.03 (0.15) Recommended								
$C_6H_{14}O$	3-Oxa-2,4-dimethylpentane (diisopropyl ether)	CAS # 108-20-3						
*1.52	D	80		SF	GLC	W	ORG	
1.52 (0.25) Recommended								
$C_6H_{14}O$	3-Oxaheptane (butylethyl ether)	CAS # 628-81-9						
*2.03	D	111		SF	GLC	W	one	46
2.03 (0.15) Recommended								
C_7H_8O	Methoxybenzene (anisole)	CAS # 100-66-3						
2.04	D	40	25	SF	AS	pH7.4	Both	117
*2.11	D	46	25	SF	AS	W	AQ	
2.08	?	150						
2.10	I	60		HPLC				
2.16[a]	I	64		HPLC				
2.24	I	57		HPLC				
2.11 (0.10) Recommended								
C_8H_6O	Benzofuran	CAS # 271-89-6						
*2.67	D	104						
2.67 (0.20) Recommended								

Table 8. Ethers (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_8H_8O	Phenylepoxyethane (styrene oxide) CAS # 96-09-3							
*1.51	D	149	37	SF	GLC	pH7.4	ORG	
*1.61	D	104						
1.84	D	151		SF	HPLC	NS	Both	
1.61 (0.20) Recommended								
C_8H_8O	2,3-Dihydrobenzofuran CAS # 496-16-2							
*2.14	D	151		SF	HPLC	NS	Both	
2.14 (0.20) Recommended								
$C_8H_{10}O$	Benzylmethyl ether CAS # 538-86-3							
*1.35	D	104						
1.35 (0.15) Recommended								
$C_8H_{10}O$	Ethoxybenzene (phenetole) CAS # 103-73-1							
*2.51	D	104						
2.68	I	57		HPLC				
2.51 (0.20) Recommended								
$C_8H_{10}O$	2-Methylanisole CAS # 578-58-5							
*2.74	D	104						
2.74 (0.20) Recommended								
$C_8H_{10}O$	3-Methylanisole CAS # 100-84-5							
*2.66	D	104						
2.66 (0.20) Recommended								
$C_8H_{10}O$	4-Methylanisole CAS # 104-93-8							
2.66	D	104						
*2.81	D	104						
2.81 (0.25) Recommended								
$C_8H_{12}O$	1-Vinyl-3,4-epoxycyclohexane							
2.08	D	149	37	SF	GLC	pH7.4	ORG	
1.90 (0.20) Recommended								

Table 8. Ethers (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{14}O$	Cyclohexylepoxyethane							
2.43	D	149	37	SF	GLC	pH7.4	ORG	
2.28	(0.20)	Recommended						
$C_8H_{18}O$	5-Oxanonane (di-n-butyl ether)				CAS # 142-96-1			
*3.21	D	152	25	SF	GLC	W	?	
3.21	(0.25)	Recommended						
$C_8H_{18}O$	4-Oxa-2,6-dimethylheptane (diisopropyl ether)						CAS # 628-55-7	
*2.78	D	80		SF	GLC	W	ORG	
2.78	(0.25)	Recommended						
$C_9H_{10}O$	Allylphenyl ether			CAS # 1746-13-0				
*2.94	D	104						
2.94	(0.30)	Recommended						
$C_9H_{12}O$	Ethylbenzyl ether			CAS # 539-30-0				
2.16	?	131						
2.16	(0.20)	Recommended						
$C_9H_{12}O$	Phenylpropyl ether			CAS # 622-85-5				
*3.18	D	104						
3.18	(0.30)	Recommended						
$C_9II_{12}O$	2,6-Dimethylanisole			CAS # 1004-66-6				
*2.92	D	104						
2.92	(0.30)	Recommended						
$C_{10}H_{14}O$	1-Methoxy-3-phenylpropane				CAS # 2046-33-5			
*2.70	D	120		SF	AS	W	AQ	46
2.70	(0.30)	Recommended						

Table 8. Ethers (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{12}H_8O$		Dibenzofuran		CAS # 132-64-9				
*4.12	D	104						
4.17	D	108	23	SF	HPLC	W	Both	
3.96	I	138		HPLC				
4.12	(0.20)	Recommended						
$C_{12}H_{10}O$		Diphenyl ether		CAS # 101-84-8				
4.08	D	108	23	SF	HPLC	W	Both	
4.20	D	135	20	SF	GLC	W	Both	
*4.21	D	104						
4.36	D	104						
3.87	I	65		HPLC				
4.21	(0.20)	Recommended						
$C_{12}H_{22}O$		1,2-Epoxycyclododecane						
4.70	I	141		HPLC				
4.57	(0.35)	Recommended						
$C_{13}H_{12}O$		Benzylphenyl ether		CAS # 946-80-5				
*3.79	D	104						
3.79	(0.30)	Recommended						

[a] Average value.

Table 9. Alcohols

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_4O	Methanol		CAS # 76-56-1					
-0.82	D	147		SF	CR	W	Both	148
*-0.77	D	104					Both	
-0.71	D	27	25	SF	GLC	pH7	Both	158
-0.70[c]	D	110		SF				
-0.68	D	154		SF	AS			
-0.66[a]	D	155				pH6		
-0.52	D	156		SF	RC	b	Both	
-0.32	D	157	34	SF	RC	pH7.4	Both	
-0.64	?	153						
-0.74	(0.07)	Recommended						
C_2H_6O	Ethanol		CAS # 64-17-5					
-0.32[a]	D	155		SF		pH6		
-0.32	D	147	20	SF	CR	W	Both	148
*-0.31	D	104					Both	
-0.30	D	159		SF	GLC	W	one	162
-0.30	D	160	25	SF	RC	W	Both	
-0.22	D	161				pH7.2		
-0.20	D	27	25	SF	GLC	pH7	Both	158
-0.18	D	156		SF	RC	b	Both	
-0.15	D	154		SF	AS			
-0.30	(0.03)	Recommended						
C_3H_4O	2-Propyn-1-ol		CAS # 107-19-7					
*-0.38	D	104						
-0.38	(0.20)	Recommended						
C_3H_6O	2-Propen-1-ol (allyl alcohol)		CAS # 107-18-6					
*0.17	D	104						
0.17	(0.10)	Recommended						
C_3H_8O	1-Propanol		CAS # 71-23-8					
*0.25	D	104					Both	
0.30	D	159		SF	GLC	W	one	162,163
0.32	D	27	25	SF	GLC	pH7	Both	158
0.25	(0.05)	Recommended						

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_3H_8O	2-Propanol		CAS # 67-63-0					
*0.05	D	159		SF	GLC	W	one	162,163
0.14	I	164		HPLC				
0.05 (0.20) Recommended								
$C_4H_{10}O$	1-Butanol		CAS # 71-36-3					
0.32?	D	157		SF	AS			
0.79	D	9,10	25	G	GLC	W	Both	11
0.79	D	58	25	G	GLC	W	Both	9
0.87	D	27	25	SF	GLC	pH7	Both	158
*0.88	D	104						
0.88^a	D	155		SF		pH6		
0.89	D	104						
0.93	D	156		SF	RC	b	Both	
0.76	I	10	25	from measured activity coefficients				
0.80	I	58	25	from measured activity coefficients				
1.02	I	165		HPLC				
0.84 (0.04) Recommended								
$C_4H_{10}O$	2-Methyl-1-propanol (isobutanol)			CAS # 78-83-1				
0.65	D	104						
*0.76	D	159		SF	GLC	W	one	162,163
0.83	D	147	20	SF	CR	W	Both	148
0.76 (0.07) Recommended								
$C_4H_{10}O$	2-Butanol		CAS # 78-92-2					
*0.61	D	111		SF	GLC	W	one	46
0.81	I	165		HPLC				
0.65 (0.10) Recommended								
$C_4H_{10}O$	2-Methyl-2-propanol (t-butyl alcohol)					CAS # 75-65-0		
*0.35	D	104					Both	
0.37	D	111		SF	GLC	W	one	46
0.39	I	164		HPLC				
0.59	I	165		HPLC				
0.35 (0.10) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_5H_8O 2-Methyl-3-butyn-2-ol CAS # 115-19-5								
*0.28	D	104						
0.28 (0.10) Recommended								
$C_5H_{12}O$ 1-Pentanol CAS # 71-41-0								
1.40	D	104						
1.49	D	27	25	SF	GLC	pH7	Both	158
1.53	D	58	25	G	GLC	W	Both	9
1.53	D	9,10	25	G	GLC	W	Both	11
*1.56	D	104					Both	
1.33	I	122		HPLC				
1.48	I	165		HPLC				
1.55	I	58	25	from measured activity coefficients				
1.51 (0.05) Recommended								
$C_5H_{12}O$ 3-Methyl-1-butanol (isopentanol) CAS # 123-51-3								
1.16	D	104						
1.42	D	104					Both	
1.16	I	164		HPLC				
1.28 (0.12) Recommended								
$C_5H_{12}O$ 2,2-Dimethyl-1-propanol CAS # 75-84-3								
1.32	D	159		SF	GLC	W	one	162,163
1.36	D	30,111		SF	GLC	W	one	46
*1.31	I	164		HPLC				
1.31 (0.05) Recommended								
$C_5H_{12}O$ 2-Pentanol CAS # 6032-29-7								
*1.19	I	164		HPLC				
1.34	I	165		HPLC				
1.25 (0.06) Recommended								
$C_5H_{12}O$ 3-Pentanol CAS # 584-02-1								
*1.21	D	104					Both	
1.09	I	164		HPLC				
1.37	I	165		HPLC				
1.21 (0.10) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_5H_{12}O$	3-Methyl-2-butanol			CAS # 598-75-4				
*1.28	D	159		SF	GLC	W	one	162,163
1.61	I	166		HPLC				
1.28 (0.20) Recommended								
$C_5H_{12}O$	2-Methyl-2-butanol			CAS # 75-85-4				
0.89	D	105		SF				
0.89	D	30	25	SF	GLC	W	AQ	46
0.89 (0.10) Recommended								
$C_5H_{12}O$	2-Ethyl-2-propanol (tert-pentanol)				CAS # 75-84-4			
*0.89	D	167		SF	AS	W	AQ	46
1.15	I	165		HPLC				
0.95 (0.10) Recommended								
C_6H_6O	Phenol		CAS # 108-95-2					
0.60?	D	169	18	SF	AS	pH6.8	AQ	
0.62?	D	172		SF	CR,AS	pH7.4	AQ	1
1.37	D	16	60	SF	CR,AS	pH2	AQ	
1.45	D	10	25	G	HPLC	W	Both	
1.46	D	86	20	SF	AS	W	AQ	46
*1.46	D	46	25	SF	AS	W	AQ	
1.48^{d}	D	168		SF				175
1.48	D	104						
1.48	D	18	22	AKUFVE				50
1.51	D	171	25	SF	AS	pH5.6	AQ	
1.51	D	16	25	SF	CR,AS	pH2	AQ	
1.54	D	50	25	AKUFVE	AS	pH 8	Both	
1.54	D	17	35	SF	AS	NS	AQ	
1.55	D	16	10	SF	CR,AS	pH2	AQ	
1.75	D	47	21	SF	AS	pH7	ORG	
1.08	I	75	25	from UNIFAC activity coefficients				
1.11	I	121		HPLC				
1.35	I	116		HPLC				
1.42^{e}	I	65		HPLC				
1.49	?	170						
1.55	?	177	25					
1.57	I	173	37	microelectrometric titration				
1.60	?	176	25			W		178
1.61	I	174		HPLC and thin-layer chromatography				
2.20	?	153						
1.50 (0.05) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_6H_{12}O$		Cyclohexanol		CAS # 108-93-0				
*1.23	D	30,111		SF	GLC	W	one	46
1.23 (0.20) Recommended								
$C_6H_{14}O$		1-Hexanol		CAS # 111-27-3				
2.02	D	152	25	SF	GLC	W	?	
2.03	D	9,10	25	G	GLC	W	Both	11
*2.03	D	104						
2.03	D	58	25	G	GLC	W	Both	9
2.04	D	27	25	SF	GLC	pH7	Both	158
1.86	I	122		HPLC				
1.99	I	165		HPLC				
2.03	I	164		HPLC				
2.05	I	58	25	from measured activity coefficients				
2.03 (0.03) Recommended								
$C_6H_{14}O$		2-Hexanol		CAS # 626-93-7				
*1.76	I	164		HPLC				
1.76 (0.20) Recommended								
$C_6H_{14}O$		3-Hexanol		CAS # 623-37-0				
*1.65	I	164		HPLC				
1.65 (0.20) Recommended								
$C_6H_{14}O$		3,3-Dimethyl-2-butanol			CAS # 464-07-3			
*1.48	D	159		SF	GLC	W	one	162,163
1.48 (0.20) Recommended								
C_7H_8O		Benzyl alcohol		CAS # 100-51-6				
1.00	D	179	20	SF	AS	NS	AQ	
1.10	D	156		SF	RC	b	Both	
1.10	D	104						
*1.10	D	30,46	25	SF	AS	W	AQ	
0.87	?	153						
1.06	I	65		HPLC				
1.05 (0.10) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_8O	2-Methylphenol		(o-cresol)		CAS # 95-48-7			
1.93	D	173	37	SF		pH7.4		
*1.95	D	104						
1.96	D	10	25	G	HPLC	W	Both	
1.97	D	104						
2.01	D	17	35	SF	AS	NS	AQ	
2.04	D	180	22	SF	CR,AS	f	AQ	
1.83	I	174		HPLC and thin-layer chromatography				
2.09	I	166		HPLC				
1.98	(0.05) Recommended							
C_7H_8O	3-Methylphenol		(m-cresol)		CAS # 108-39-4			
1.94	D	173	37	SF		pH7.4		
1.95^d	D	168		SF				175
*1.96	D	46	25	SF	AS	W	AQ	
1.96	D	9,10	25	G	HPLC	W	Both	
2.01	D	104						
2.06	D	17	35	SF	AS	NS	AQ	
1.94	I	174		HPLC				
2.01	?	181						
1.98	(0.08) Recommended							
C_7H_8O	4-Methylphenol		(p-cresol)		CAS # 106-44-5			
1.91	D	173	37	SF		pH7.4		
1.92	D	104						
*1.94	D	46	25	SF	AS	W	AQ	
1.95^d	D	168		SF				175
1.98	D	18	22	SF	AS		Both	50
1.99	D	171	25	SF	AS	pH5.6	AQ	
2.10	D	17	35	SF	AS	NS	AQ	
1.62	I	57		HPLC				
1.73	I	75	25	from UNIFAC activity coefficients				
1.97	I	166		HPLC				
2.03	I	174		HPLC				
2.10	?	177	25					
2.17	?	181						
1.97	(0.07) Recommended							
$C_7H_{14}O$	cis-2-Methylcyclohexanol				CAS # 7443-70-1			
*1.84	I	164		HPLC				
1.84	(0.10) Recommended							

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_7H_{14}O$ trans-2-Methylcyclohexanol CAS # 7443-52-9								
*1.82	I	164		HPLC				
1.82 (0.10) Recommended								
$C_7H_{14}O$ 4-Methylcyclohexanol CAS # 589-91-3								
*1.79	D	104						
1.79 (0.15) Recommended								
$C_7H_{16}O$ 1-Heptanol CAS # 111-70-6								
2.57	D	9,10	25	G	GLC	W	Both	
2.57	D	58	25	G	GLC	W	Both	9
2.60	D	164	25	G	GLC	W	Both	11
2.65	D	27	25	SF	GLC	pH7	Both	158
*2.72	D	104						
2.39	I	122		HPLC				
2.41	I	165		HPLC				
2.62 (0.10) Recommended								
$C_7H_{16}O$ 2-Heptanol CAS # 543-49-7								
*2.31	D	104						
2.31 (0.20) Recommended								
$C_7H_{16}O$ 3-Heptanol CAS # 589-82-2								
*2.24	D	104						
2.24 (0.20) Recommended								
$C_7H_{16}O$ 4-Heptanol CAS # 589-55-9								
*2.22	D	104						
2.13	I	164		HPLC				
2.22 (0.10) Recommended								
$C_8H_{10}O$ 3-Methylbenzyl alcohol CAS # 587-03-1								
*1.60	D	46	25	SF	AS	W	AQ	
1.60 (0.15) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{10}O$		4-Methylbenzyl alcohol			CAS # 589-18-4			
*1.58	D	46	25	SF	AS	W	AQ	
1.59	D	104						
1.58	(0.15)	Recommended						
$C_8H_{10}O$		2-Ethylphenol		CAS # 90-00-6				
*2.47	D	104						
2.64	?	181						
2.64	I	174		HPLC				
2.47	(0.15)	Recommended						
$C_8H_{10}O$		3-Ethylphenol		CAS # 620-17-7				
*2.40	D	46	25	SF	AS	W	AQ	
2.47	?	181						
2.59	I	174		HPLC				
2.50	(0.10)	Recommended						
$C_8H_{10}O$		4-Ethylphenol		CAS # 123-07-9				
*2.58	D	171	25	SF	AS	pH5.6	AQ	
2.60	D	17	35	SF	AS	NS	AQ	
2.26	?	170						
2.37	I	174		HPLC				
2.59	?	177	25					
2.50	(0.10)	Recommended						
$C_8H_{10}O$		1-Phenylethanol		CAS # 1517-69-7				
*1.42	D	104						
1.42	(0.15)	Recommended						
$C_8H_{10}O$		2-Phenylethanol		CAS # 60-12-8				
1.29	D	179	20	SF	AS	NS	AQ	
*1.36	D	120		SF	AS	W	AQ	46
1.36	(0.10)	Recommended						

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{10}O$		2,4-Dimethylphenol		CAS # 105-67-9				
*2.30	D	182	20	SF	CR,AS	pH2	AQ	183
2.34	D	10	25	G	HPLC	W	Both	
2.42	D	108	23	SF	RC	W	Both	
2.54	D	17	35	SF	AS	NS	AQ	
2.35 (0.15) Recommended								
$C_8H_{10}O$		2,5-Dimethylphenol		CAS # 95-87-4				
*2.33	D	182	20	SF	CR,AS	pH2	AQ	183
2.35	D	10	25	G	HPLC	W	Both	
2.34 (0.15) Recommended								
$C_8H_{10}O$		2,6-Dimethylphenol		CAS # 576-26-1				
2.27	D	104						
2.31	D	10	25	G	HPLC	W	Both	
*2.36	D	104						
2.40	D	17	35	SF	AS	pH2	AQ	
2.07	I	57		HPLC				
2.38	I	166		HPLC				
2.36 (0.10) Recommended								
$C_8H_{10}O$		3,4-Dimethylphenol		CAS # 95-65-8				
*2.23	D	182	20	SF	CR,AS	pH2	AQ	183
2.23 (0.25) Recommended								
$C_8H_{10}O$		3,5-Dimethylphenol		CAS # 108-68-9				
*2.35	D	104						
2.55	D	17	35	SF	AS	NS	AQ	
2.31	?	170						
2.38	I	75	25	from UNIFAC activity coefficients				
2.35 (0.15) Recommended								
$C_8H_{16}O$		α,α,α-2,6-Dimethylcyclohexanol		CAS # 39170-84-8				
*2.37	I	164		HPLC				
2.37 (0.25) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{16}O$ α, α, β-2,6-Dimethylcyclohexanol CAS # 39170-83-7								
*2.10	I	164		HPLC				
2.10 (0.25) Recommended								
$C_8H_{16}O$ α, β, β-2,6-Dimethylcyclohexanol CAS # 42846-29-7								
*2.38	I	164		HPLC				
2.38 (0.25) Recommended								
$C_8H_{18}O$ 1-Octanol CAS # 111-87-5								
3.15	D	147	25	SF	CR	W	AQ	148
3.16	D	184	23	SF		W	AQ	
3.27	D	27	25	SF	GLC	pH7	Both	158
2.80	I	165		HPLC				
2.92	I	122		HPLC				
*2.97	I	112		HPLC				
3.07 (0.10) Recommended								
$C_8H_{18}O$ 2-Octanol CAS # 123-96-6								
*2.90	I	164		HPLC				
2.90 (0.25) Recommended								
$C_8H_{18}O$ 4-Octanol CAS # 589-62-8								
*2.68	I	164		HPLC				
2.68 (0.25) Recommended								
$C_9H_{10}O$ 3-Phenyl-2-propen-1-ol (cinnamyl alcohol) CAS # 104-54-1								
*1.95	D	104						
1.78	I	57		HPLC				
1.95 (0.20) Recommended								
$C_9H_{12}O$ 3-Phenyl-1-propanol CAS # 122-97-4								
1.85	D	179	20	SF	AS	NS	AQ	
*1.88	D	120		SF	AS	W	AQ	46
1.88 (0.10) Recommended								

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{12}O$		2-n-Propylphenol		CAS # 644-35-9				
*2.93	D	104						
2.93	(0.25)	Recommended						
$C_9H_{12}O$		4-n-Propylphenol		CAS # 645-56-7				
*3.20	D	17	35	SF	AS	NS	AQ	
3.21	?	177	25					
3.20	(0.10)	Recommended						
$C_9H_{12}O$		2-Isopropylphenol		CAS # 88-69-7				
*2.88	D	104						
2.88	(0.20)	Recommended						
$C_9H_{12}O$		2,3,6-Trimethylphenol		CAS # 2416-94-6				
2.67	D	10	25	G	HPLC	W	Both	
2.67	(0.35)	Recommended						
$C_9H_{12}O$		2,4,6-Trimethylphenol		CAS # 527-60-6				
2.73	D	10	25	G	HPLC	W	Both	
2.73	(0.35)	Recommended						
$C_9H_{20}O$		1-Nonanol		CAS # 143-08-8				
3.77	D	9,10	25	G	GLC	W	Both	11
*4.26	D	104						
4.02	(0.30)	Recommended						
$C_{10}H_8O$		1-Naphthol		CAS # 90-15-3				
2.31	D	185	20	SF	CR,AS	f	AQ	
*2.84	D	172		SF	FL	pH7.4		1
2.98	D	111		SF	AS	W	AQ	46
3.09	D	186		SF	g	pH6.5	AQ	
2.28	I	57		HPLC				
2.84	(0.20)	Recommended						

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_8O$		2-Naphthol		CAS # 135-19-3				
*2.70	D	187		SF	AS	f	Both	46
2.84	D	111		SF	AS	W	one	46
2.89	D	185	20	SF	CR,AS	f	AQ	
2.46^{e}	I	65		HPLC				
2.70 (0.15)	Recommended							
$C_{10}H_{14}O$		4-n-Butylphenol		CAS # 1638-22-8				
3.65	D	17	20	SF	AS	NS	AQ	
3.65 (0.20)	Recommended							
$C_{10}H_{14}O$		4-tert-Butylphenol		CAS # 98-54-4				
3.04^{c,h}	D	110		SF				
3.04 (0.40)	Recommended							
$C_{10}H_{20}O$		cis-4-tert-Butylcyclohexanol		CAS # 937-05-3				
*3.02	I	164		HPLC				
3.02 (0.40)	Recommended							
$C_{10}H_{20}O$		trans-4-tert-Butylcyclohexanol		CAS # 21862-63-5				
*3.09	I	164		HPLC				
3.09 (0.40)	Recommended							
$C_{10}H_{22}O$		1-Decanol		CAS # 112-30-1				
*4.57	D	104						
3.98	I	122		HPLC				
4.57 (0.50)	Recommended							
$C_{12}H_{26}O$		1-Dodecanol		CAS # 112-53-8				
*5.13	D	104						
5.24	D	132		SF	GLC	pH7	Both	
5.04	I	122		HPLC				
5.13 (0.30)	Recommended							

Table 9. Alcohols (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{13}H_{10}O$		7-Phenyl-4,6-diyn-hept-2-en-1-ol				CAS # 13641-62-8		
2.48	I	145		HPLC				
2.48 (0.50) Recommended								
$C_{13}H_{12}O$		Diphenylmethanol		CAS # 91-01-0				
2.03	D	104						
*2.67	D	125		SF				1
2.67	D	104						
2.67 (0.25) Recommended								
$C_{14}H_{14}O$		Phenyl-2-methylphenylmethanol			CAS # 5472-13-9			
*3.06	D	104						
3.06 (0.30) Recommended								
$C_{14}H_{14}O$		Phenyl-4-methylphenylmethanol			CAS # 1517-63-1			
*3.13	D	104						
3.13 (0.30) Recommended								
$C_{14}H_{22}O$		2,6-Di-sec-butylphenol		CAS # 5510-99-6				
4.38	I	104		HPLC				
4.4 (1.0) Recommended								
$C_{19}H_{16}O$		Triphenylmethanol		CAS # 76-84-6				
*3.68	D	104						
3.68 (0.40) Recommended								

[a] J. Y. Park, unpublished data.

[b] Schistosome saline solution.

[c] D. Kotzias, personal communication.

[d] K. Thomae, personal communication.

[e] From a restricted correlation plot.

[f] "Acidified".

[g] Chemical reaction followed by density measurement.

[h] Average value.

Table 10. Aldehydes

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_2O	Methanal (formaldehyde)	CAS # 50-00-0						
*0.35	D	188	25	SF	CR	W	Both	
0.35	(0.10)	Recommended						
C_2H_4O	Ethanal (acetaldehyde)	CAS # 75-07-0						
0.52	D	10	25	G	HPLC	W	Both	
0.45	(0.10)	Recommended						
C_3H_4O	Propenal (acrolein)	CAS # 107-02-8						
-0.01	D	104						
-0.01	(0.25)	Recommended						
C_3H_6O	Propanal	CAS # 123-38-6						
*0.59	D	104						
0.59	(0.20)	Recommended						
C_4H_8O	Butanal	CAS # 123-72-8						
*0.88	D	104						
0.88	(0.20)	Recommended						
C_5H_8O	2-Ethylpropenal	CAS # 922-63-4						
*1.24	D	104						
1.24	(0.20)	Recommended						
$C_6H_{12}O$	Hexanal	CAS # 66-25-1						
*1.78	D	189	25	SF	GLC	pH7	AQ	46
1.78	(0.15)	Recommended						

Table 10. Aldehydes (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_6O		Benzaldehyde		CAS # 100-52-7				
1.43	D	190	25	SF	AS	W	ORG	191
1.45	D	171	25	SF	AS	pH5.6	AQ	
*1.48	D	104						
1.44[a]	I	64		HPLC				
1.56	I	65		HPLC				
2.33	I	56		HPLC				
1.48	(0.08)	Recommended						
C_8H_8O		Phenylethanal		CAS # 122-78-1				
*1.78	D	104						
1.78	(0.25)	Recommended						
C_8H_8O		2-Methylbenzaldehyde			CAS # 529-20-4			
*2.26	D	192	AMB	SF	AS	W	AQ	
2.26	(0.20)	Recommended						
$C_{13}H_8O$		7-Phenylhept-2-ene-4,6-diynal				CAS # 20252-42-0		
3.09	I	145		HPLC				112,146
3.1	(1.0)	Recommended						

[a] Average value.

Table 11. Ketones

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_3H_6O		2-Propanone (acetone)			CAS # 67-64-1			
-0.48	D	193		SF	GLC	W	AQ	194
*-0.24	D	147	20	SF	CR	W	Both	148
-0.24	(0.10)	Recommended						
C_4H_8O		2-Butanone (methylethyl ketone)				CAS # 78-93-3		
0.26	D	147	20	SF	CR	W	Both	148
0.26	D	193		SF	GLC	W	AQ	194
*0.29	D	30,111		SF	AS,GLC	W	one	46
0.50	D	104				D_2O		
0.69?	D	9,10	25	G	GLC	W	Both	11
0.29	(0.05)	Recommended						
$C_5H_{10}O$		2-Pentanone		CAS # 107-87-9				
0.78	D	193		SF	GLC	W	AQ	194
*0.91	D	189	25	SF	AS	pH7	AQ	46
0.84	(0.08)	Recommended						
$C_5H_{10}O$		3-Pentanone (diethyl ketone)			CAS # 96-22-0			
0.99	D	9,10	25	G	GLC	W	Both	11
0.67	I	22	25	from measured activity coefficients				
0.75	I	10	25	from measured activity coefficients				
0.82	(0.15)	Recommended						
$C_5H_{10}O$		3-Methyl-2-butanone			CAS # 563-80-4			
*0.56	D	193		SF	GLC	W	AQ	194
0.56	(0.10)	Recommended						
C_6H_8O		1-Hexyn-5-one		CAS # 2550-28-9				
*0.58	D	104						
0.58	(0.15)	Recommended						
C_6H_8O		2-Cyclohexene-1-one			CAS # 930-68-7			
*0.61	D	104						
0.61	(0.15)	Recommended						

Table 11. Ketones (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_6H_{10}O$		1-Hexen-5-one		CAS # 109-49-9				
*1.02	D	120		SF	AS	W	AQ	46
1.02	(0.10)	Recommended						
$C_6H_{10}O$		Cyclohexanone		CAS # 108-94-1				
*0.81	D	104						
0.81	(0.15)	Recommended						
$C_6H_{12}O$		2-Hexanone		CAS # 591-78-6				
1.19	D	193		SF	GLC	W	AQ	194
*1.38	D	120		SF	AS	W	AQ	46
1.39	I	57		HPLC				
1.38	(0.20)	Recommended						
$C_6H_{12}O$		4-Methyl-2-pentanone		CAS # 108-10-1				
*1.31	D	193		SF	GLC	W	AQ	194
1.31	(0.20)	Recommended						
$C_7H_{14}O$		2-Heptanone		CAS # 110-43-0				
*1.98	D	9,10	25	G	HPLC	W	Both	11
2.03	D	193		SF	GLC	W	AQ	194
2.08	I	10	25	from measured activity coefficients				
1.98	(0.15)	Recommended						
$C_7H_{14}O$		5-Methyl-2-hexanone		CAS # 110-12-3				
*1.88	D	193		SF	GLC	W	AQ	194
1.88	(0.15)	Recommended						

Table 11. Ketones (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_8H_8O		Acetophenone		CAS # 98-86-2				
*1.58	D	46	25	SF	AS	W	AQ	
1.58	D	118	23	SF	HPLC	W	Both	
1.59	D	197	AMB	SF	RC	W	Both	
1.63	D	92		SF				
1.68	D	190	25	SF	AS	W	ORG	191
1.73	D	195		SF	AS	W	AQ	46
1.58	I	196		HPLC				
1.59	?	198						
1.65	I	92		HPLC				
1.71[a]	I	64		HPLC				
1.72	I	65		HPLC				
1.80	I	121		HPLC				
1.63	(0.05)	Recommended						
$C_8H_{16}O$		2-Octanone		CAS # 111-13-7				
*2.37	D	193		SF	GLC	W	AQ	194
2.76	D	9,10	25	G	HPLC	W	Both	11
2.37	(0.10)	Recommended						
C_9H_8O		Acrylophenone		CAS # 768-03-6				
*1.88	D	104						
1.88	(0.30)	Recommended						
$C_9H_{10}O$		Propiophenone		CAS # 93-55-0				
*2.19	D	104						
2.21	D	190	25	SF	AS	W	ORG	191
2.16	I	57		HPLC				
2.19	(0.10)	Recommended						
$C_9H_{10}O$		4-Methylacetophenone		CAS # 122-00-9				
2.28	D	195		SF	AS	W	AQ	46
*2.10	I	196		HPLC				
2.19	(0.10)	Recommended						

Table 11. Ketones (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{10}O$		1-Phenyl-2-propanone		CAS # 103-79-7				
*1.44	D	120		SF	AS	W	AQ	46
1.17[a]	I	64		HPLC				
1.44 (0.10)	Recommended							
$C_9H_{18}O$		2-Nonanone		CAS # 821-55-6				
3.14	D	193		SF	GLC	W	AQ	194
3.18	D	9,10	25	G	HPLC	W	Both	11
3.16 (0.20)	Recommended							
$C_9H_{18}O$		5-Methyl-2-octanone		CAS # 58654-67-4				
2.92	D	193		SF	GLC	W	AQ	194
2.92 (0.20)	Recommended							
$C_{10}H_{10}O$		4-Phenyl-3-buten-2-one (methylstyryl ketone)				CAS # 122-57-6		
*2.07	?	199						
2.07 (0.30)	Recommended							
$C_{10}H_{20}O$		2-Decanone		CAS # 693-54-9				
3.73	D	193		SF	GLC	W	AQ	194
3.81	D	9,10	25	G	HPLC	W	Both	11
3.77 (0.40)	Recommended							
$C_{11}H_{14}O$		4-Isopropylacetophenone		CAS # 645-13-6				
2.98	I	196		thin-layer chromatography				
2.98 (0.30)	Recommended							
$C_{11}H_{22}O$		2-Undecanone		CAS # 112-12-9				
4.09	D	193		SF	GLC	W	AQ	194
4.09 (0.30)	Recommended							
$C_{12}H_{10}O$		1-Acetylazulene		CAS # 7206-57-7				
*2.87	D	127		SF	AS	W	ORG	3
2.87 (0.25)	Recommended							

Table 11. Ketones (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{12}H_{14}O$		4-Phenylcyclohexanone		CAS # 4894-75-1				
2.30	I	143		HPLC				
2.45	(0.25)	Recommended						
$C_{12}H_{22}O$		Cyclododecanone		CAS # 830-13-7				
4.10	I	141		HPLC				
4.10	(0.40)	Recommended						
$C_{13}H_8O$		9-Fluorenone		CAS # 486-25-9				
*3.58	D	104						
3.58	(0.30)	Recommended						
$C_{13}H_{10}O$		Benzophenone		CAS # 119-61-9				
3.12	D	104						
*3.18	D	104						
3.58	D	190	25	SF	AS	W	ORG	191
3.18	(0.20)	Recommended						
$C_{14}H_{12}O$		2-Phenylacetophenone		CAS # 451-40-1				
*3.18	D	104						
3.18	(0.25)	Recommended						

[a] Average value.

Table 12. Acids

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_2O_2 Methanoic (formic) acid CAS # 64-18-6 $pK_a = 3.74$								
*-0.54	D	147	20	SF	T	W	Both	148
-0.54	D	200	25	SF	T	W	Both	
-0.54 (0.20) Recommended								
$C_2H_4O_2$ Ethanoic (acetic) acid CAS # 64-19-7 $pK_a = 4.76$								
-0.31	D	147	20	SF	T	W	Both	148
-0.30	D	201	28	SF	T	W	Both	
-0.29	D	202	25	SF	RC	pH1		
*-0.17	D	104						
-0.24[a]	?	173	37					
-0.17 (0.20) Recommended								
$C_3H_6O_2$ Propanoic acid CAS # 79-09-4 $pK_a = 4.87$								
0.25	D	147	20	SF	T	W	Both	148
0.27	D	203		SF	T	W	AQ	204
*0.33	D	104						
0.32[a]	?	173	37					
0.33 (0.10) Recommended								
$C_4H_6O_2$ 2-Butenoic (crotonic) acid (isomer not specified) CAS # 3724-65-0 $pK_a \sim 4.5$								
*0.72	D	104						
0.72	D	104						
0.66[a]	?	173						
0.72 (0.15) Recommended								
$C_4H_6O_2$ 2-Methylpropenoic (methacrylic) acid CAS # 79-41-4 $pK_a = 4.66$								
*0.93	D	205	22	SF	T	W	AQ	
0.93 (0.20) Recommended								
$C_4H_8O_2$ Butanoic acid CAS # 107-92-6 $pK_a = 4.82$								
*0.79	D	147	20	SF	T	W	Both	148
0.83[a]	?	173	37					
0.98	?	206						
0.79 (0.10) Recommended								

Table 12. Acids (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_5H_{10}O_2$	Pentanoic acid			CAS # 109-52-4		pK$_a$ = 4.83		
*1.39[a]	?	173	37					
1.51	?							
1.39 (0.15) Recommended								
$C_6H_8O_2$	2,4-Hexadienoic (sorbic) acid				CAS # 110-44-1		pK$_a$ = 4.6 (est.)	
*1.33[a]	?	173	37					
1.33 (0.25) Recommended								
$C_6H_{12}O_2$	Hexanoic (caproic) acid			CAS # 142-62-1		pK$_a$ = 4.87		
1.88	D	104						
*1.92	D	104						
1.92	D	203		SF	T	W	AQ	204
2.09	D	207	25	SF	FL	pH0.5	AQ	
1.87	I	122		HPLC				
1.93	?	206						
2.07[a]	?	173	37					
1.92 (0.15) Recommended								
$C_6H_{12}O_2$	2-Methylpentanoic acid			CAS # 97-61-0		pK$_a$ = 4.79 (18°C)		
*1.80	?	206						
1.80 (0.15) Recommended								
$C_6H_{12}O_2$	2-Ethylbutanoic acid			CAS # 88-09-5		pK$_a$ = 4.74		
*1.68	?	206						
1.68 (0.20) Recommended								
$C_7H_6O_2$	Benzoic acid			CAS # 65-85-0		pK$_a$ = 4.20		
1.24?	D	210	25	SF	AS	pH1	AQ	
1.68	D	208	25	SF	AS	W	Both	
*1.87	D	46	25	SF	AS	W	AQ	
1.88	D	207	25	SF	AS	pH0.5	AQ	
1.94	D	211		SF	RC	pH0.5	Both	

Table 12. Acids (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_7H_6O_2$	Benzoic acid (continued)							
1.47	I	37	25	from solubility ratio				
1.71^a	?	173	37					
1.87	I	44	25	microelectrometric titration				
1.97	I	209	25	microelectrometric titration				
2.03	?	150						
1.87 (0.10) Recommended								
$C_8H_8O_2$	Phenylethanoic acid			CAS # 103-82-2		$pK_a = 4.31$		
1.18?	D	214	25	SF	b	W	Both	
*1.41	D	46	25	SF	AS	W	AQ	
1.45	D	213	25	SF	AS	pH3.5	Both	
1.51	D	154		SF	AS			
1.45^a	?	173	37					
1.95?	I	123		HPLC				
1.41 (0.15) Recommended								
$C_8H_8O_2$	2-Methylbenzoic acid			CAS # 118-90-1		$pK_a = 3.92$		
2.18	D	215	25	SF	AS	W	AQ	
*2.46	D	104				pH1		
2.46 (0.20) Recommended								
$C_8H_8O_2$	3-Methylbenzoic acid			CAS # 99-04-7		$pK_a = 4.27$		
*2.37	D	46	25	SF	AS	W	AQ	
2.37 (0.20) Recommended								
$C_8H_8O_2$	4-Methylbenzoic acid			CAS # 99-94-5		$pK_a = 4.39$		
*2.27	D	46	25	SF	AS	W	AQ	
2.36	D	71	23	SF	AS	pH2.3	ORG	
2.34	I	44	25	microelectrometric titration				
2.67?	I	123		HPLC				
2.34 (0.20) Recommended								

Table 12. Acids (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{16}O_2$	Octanoic (caprylic) acid			CAS # 124-07-2		$pK_a = 4.89$		
2.93	I	122		HPLC				
*3.05^a	?	173						
3.05 (0.20)	Recommended							
$C_8H_{16}O_2$	2-Ethylhexanoic acid			CAS # 149-57-5		$pK_a = 4.8$ (est.)		
*2.64	?	206						
2.64 (0.25)	Recommended							
$C_8H_{16}O_2$	2-Propylpentanoic acid			CAS # 99-66-1		$pK_a = 4.8$ (est.)		
0.13^c	D	104				pH7.5		
*2.75	?	206						
2.75 (0.25)	Recommended							
$C_9H_8O_2$	3-Phenyl-2-propenoic (cinnamic) acid (isomer not specified)				CAS # 621-82-9	$pK_a \sim 4.2$		
2.08	D	154		SF	AS			
2.37	D	104				pH1		
2.41^a	?	173	37					
2.25 (0.25)	Recommended							
$C_9H_8O_2$	trans-3-Phenyl-2-propenoic acid			CAS # 140-10-3		$pK_a = 4.44$		
*2.13	D	104						
2.39	I	216		HPLC				
2.13 (0.20)	Recommended							
$C_9H_{10}O_2$	2-Phenylpropanoic acid			CAS # 492-37-5		$pK_a = 4.7$ (est.)		
1.80^c	D	213	25	SF	AS	pH3.5	Both	
1.80 (0.20)	Recommended							
$C_9H_{10}O_2$	3-Phenylpropanoic acid			CAS # 501-52-0		$pK_a = 4.66$		
*1.84	D	120		SF	AS	W	AQ	46
1.91	D	213	25	SF	AS	pH3.5	Both	
1.84 (0.15)	Recommended							

Table 12. Acids (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{10}O_2$ 3-Methylphenylethanoic acid CAS # 621-36-3 pK_a= 4.4 (est.)								
*1.95	D	46	25	SF	T	W	AQ	
1.95 (0.20) Recommended								
$C_9H_{10}O_2$ 4-Methylphenylethanoic acid CAS # 622-47-9 pK_a= 4.37								
*1.86	D	46	25	SF	AS	W	AQ	
1.86 (0.20) Recommended								
$C_9H_{18}O_2$ 2-Propylhexanoic acid CAS # 3274-28-0 pK_a= 4.7 (est.)								
*3.01	?	206						
3.01 (0.30) Recommended								
$C_{10}H_{10}O_2$ 2-Methyl-3-phenylpropenoic acid CAS # 1199-77-5 pK_a= 4.4 (est.)								
2.89	I	216		HPLC				
2.60 (0.35) Recommended								
$C_{10}H_{20}O_2$ Decanoic (capric) acid CAS # 334-48-5 pK_a= 4.9 (est.)								
*4.09	D	104						
3.99	I	122		HPLC				
4.09[a]	?	173						
4.09 (0.30) Recommended								
$C_{10}H_{20}O_2$ 2-Propylheptanoic acid CAS # 31080-39-4 pK_a= 4.7 (est.)								
*3.20	?	206						
3.55 (0.40) Recommended								
$C_{10}H_{20}O_2$ 2-Butylhexanoic acid CAS # 3115-28-4 pK_a= 4.7 (est.)								
*3.20	?	206						
3.55 (0.40) Recommended								

Table 12. Acids (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{11}H_{10}O_2$ 5-Phenyl-2,4-pentadienoic acid CAS # 1552-94-9 $pK_a = 4.3$ (est.)								
3.15	I	216		HPLC				
2.5 (0.5) Recommended								
$C_{12}H_{24}O_2$ Dodecanoic (lauric) acid CAS # 143-07-7 $pK_a = 5.3$ (20°C)								
*4.20	D	104						
5.05	I	122		HPLC				
4.6 (0.5) Recommended								
$C_{14}H_{12}O_2$ Diphenylethanoic acid CAS # 117-34-0 $pK_a = 3.94$								
*2.17	D	212		SF	AS	W	AQ	
*3.09	D	104				pH1		
2.6 (0.5) Recommended								
$C_{14}H_{28}O_2$ Tetradecanoic (myristic) acid CAS # 544-63-8 $pK_a = 4.5$ (est.)								
6.11	I	122		HPLC				
6.1 (0.6) Recommended								
$C_{15}H_{10}O_2$ Anthracene-9-carboxylic acid CAS # 723-62-6 $pK_a = 3.65$ (20°C)								
3.11	D	217		SF	RC	W	Both	134
4.3 (0.5) Recommended								
$C_{16}H_{30}O_2$ 8-Hexadecenoic (palmitoleic) acid (isomer not specified) CAS # 17004-62-5 $pK_a = 4.5$ (est.)								
6.58	I	122		HPLC				
6.58 (0.65) Recommended								
$C_{16}H_{32}O_2$ Hexadecanoic (palmitic) acid CAS # 57-10-3 $pK_a = 4.5$ (est.)								
7.17	I	122		HPLC				
7.17 (0.70) Recommended								

Table 12. Acids (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{18}H_{30}O_2$ 9,12,15-Octadecatrienoic (linolenic) acid CAS # 463-40-1 pK$_a$= 4.5 (est.)								
6.46	I	122		HPLC				
6.46 (0.65)	Recommended							
$C_{18}H_{32}O_2$ 9,12-Octadecadienoic (linoleic) acid CAS # 60-33-3 pK$_a$= 4.77								
7.05	I	122		HPLC				
7.05 (0.70)	Recommended							
$C_{18}H_{34}O_2$ 9-Octadecenoic (oleic) acid (isomer not specified) CAS # 2027-47-6 pK$_a$= 4.5 (est.)								
7.64	I	122		HPLC				
7.64 (0.76)	Recommended							
$C_{18}H_{36}O_2$ Octadecanoic (stearic)acid CAS # 57-11-4 pK$_a$= 4.5 (est.)								
8.23	I	122		HPLC				
8.23 (0.82)	Recommended							
$C_{20}H_{32}O_2$ 5,8,11,14-eicosatetraenoic (arachidonic) acid CAS # 506-32-1 pK$_a$= 4.5 (est.)								
6.98	I	122		HPLC				
6.98 (0.70)	Recommended							
$C_{20}H_{40}O_2$ Eicosanoic acid CAS # 506-30-9 pK$_a$= 4.5 (est.)								
9.29	I	122		HPLC				
9.29 (0.93)	Recommended							

[a] From an unidentified literature source.

[b] RC or AS or T.

[c] Not ion-corrected.

Table 13. Esters

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_4H_8O_2$	Methanoic acid, n-propyl ester				CAS # 110-74-7			
*0.83	D	104						
0.83 (0.15) Recommended								
$C_7H_6O_2$	Methanoic acid, phenyl ester				CAS # 1864-94-4			
*1.26	I	60		HPLC				
1.26 (0.30) Recommended								
$C_3H_6O_2$	Ethanoic acid, methyl ester				CAS # 79-20-9			
*0.18	D	147	20	SF	CR	W	Both	148
0.18 (0.05) Recommended								
$C_4H_6O_2$	Ethanoic acid, vinyl ester				CAS # 108-05-4			
0.60	D	218		SF				
*0.73	D	104						
0.21?	I	144		HPLC				
0.73 (0.15) Recommended								
$C_4H_8O_2$	Ethanoic acid, ethyl ester				CAS # 141-78-6			
0.66	D	147	20	SF	CR	W	Both	148
0.68	D	9,10	25	G	GLC	W	Both	11
*0.73	D	30,111		SF	GLC	W	one	46
0.53	I	10	25	from measured activity coefficients				
0.73 (0.05) Recommended								
$C_5H_{10}O_2$	Ethanoic acid, n-propyl ester				CAS # 109-60-4			
1.24	D	9,10	25	G	GLC	W	Both	11
1.11	I	10	25	from measured activity coefficients				
1.24 (0.15) Recommended								
$C_6H_{12}O_2$	Ethanoic acid, n-butyl ester				CAS # 123-86-4			
1.82	D	9,10	25	G	GLC	W	Both	11
1.69	I	10	25	from measured activity coefficients				
1.82 (0.15) Recommended								

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_8O_2$	Ethanoic acid, phenyl ester CAS # 122-79-2							
*1.49	D	46	25	SF	AS	W	AQ	
1.49 (0.20) Recommended								
$C_9H_{10}O_2$	Ethanoic acid, benzyl ester CAS # 140-11-4							
*1.96	D	120		SF	AS	W	AQ	46
1.99	D	219	25	SF	AS	W	AQ	46
1.96 (0.15) Recommended								
$C_9H_{10}O_2$	Ethanoic acid, 2-methylphenyl ester CAS # 533-18-6							
*1.93	D	104						
2.11	D	192	AMB	SF	AS	W	AQ	
1.93 (0.20) Recommended								
$C_9H_{10}O_2$	Ethanoic acid, 3-methylphenyl ester CAS # 122-46-3							
*2.09	D	192	AMB	SF	AS	W	AQ	
2.09 (0.20) Recommended								
$C_9H_{10}O_2$	Ethanoic acid, 4-methylphenyl ester CAS # 140-39-6							
*2.11	D	192	AMB	SF	AS	W	AQ	
2.11 (0.20) Recommended								
$C_{10}H_{12}O_2$	Ethanoic acid, 2-phenylethyl CAS # 103-45-7							
*2.30	D	120		SF	AS	W	AQ	46
2.30 (0.25) Recommended								
$C_{10}H_{12}O_2$	Ethanoic acid, 4-ethylphenyl ester CAS # 3245-23-6							
*2.56	D	104						
2.56 (0.25) Recommended								
$C_{10}H_{12}O_2$	Ethanoic acid, 2-ethylphenyl ester CAS # 3056-59-5							
*2.42	D	104						
2.42 (0.30) Recommended								

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_{12}O_2$	Ethanoic acid, 4-methylbenzyl ester CAS# 2216-45-7							
*2.44	D	219	25	SF	AS	W	AQ	
2.44	(0.25)	Recommended						
$C_4H_6O_2$	Propenoic acid, methyl ester CAS # 96-33-3							
*0.80	D	194	AMB	SF	GLC	W	AQ	
0.36?	I	144		HPLC				
0.80	(0.15)	Recommended						
$C_5H_8O_2$	Propenoic acid, ethyl ester CAS # 140-88-5							
*1.32	D	104						
*1.33	D	194	AMB	SF	GLC	W	AQ	
0.66?	I	144		HPLC				
1.32	(0.15)	Recommended						
$C_7H_{12}O_2$	Propenoic acid, n-butyl ester CAS # 141-32-2							
*2.36	D	194	AMB	SF	GLC	W	AQ	
1.67?	I	144		HPLC				
2.36	(0.25)	Recommended						
$C_7H_{12}O_2$	Propenoic acid, isobutyl ester CAS # 106-63-8							
*2.22	D	194	AMB	SF	GLC	W	AQ	
2.22	(0.25)	Recommended						
$C_5H_{10}O_2$	Propanoic acid, ethyl ester CAS # 105-37-3							
*1.21	D	111		SF	GLC	W	one	46
1.43	D	9,10	25	G	GLC	W	Both	11
1.60	I	57		HPLC				
1.21	(0.15)	Recommended						

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_5H_8O_2$ 2-Methylpropenoic acid, methyl ester CAS # 80-62-6								
0.70?	D	144		SF				
*1.38	D	194	AMB	SF	GLC	W	AQ	
0.67?	I	144		HPLC				
1.38 (0.15) Recommended								
$C_6H_{10}O_2$ 2-Methylpropenoic acid, ethyl ester CAS # 97-63-2								
1.30?	D	144		SF				
*1.94	D	194	AMB	SF	GLC	W	AQ	
1.25?	I	144		HPLC				
1.94 (0.20) Recommended								
$C_7H_{12}O_2$ 2-Methylpropenoic acid, isopropyl ester CAS # 4655-34-9								
*2.25	D	194	AMB	SF	GLC	W	AQ	
2.25 (0.25) Recommended								
$C_8H_{14}O_2$ 2-Methylpropenoic acid, n-butyl ester CAS # 97-88-1								
2.60	D	144		SF				
*2.88	D	194	AMB	SF	GLC	W	AQ	
2.26?	I	144		HPLC				
2.88 (0.30) Recommended								
$C_8H_{14}O_2$ 2-Methylpropenoic acid, isobutyl ester CAS # 97-86-9								
*2.66	D	194	AMB	SF	GLC	W	AQ	
2.01?	I	144		HPLC				
2.66 (0.25) Recommended								
$C_8H_{14}O_2$ 2-Methylpropenoic acid, tert-butyl ester CAS # 585-07-9								
*2.54	D	194	AMB	SF	GLC	W	AQ	
2.01?	I	144		HPLC				
2.54 (0.25) Recommended								

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_{16}O_2$	2-Methylpropenoic acid, cyclohexyl ester CAS # 101-43-9							
3.96	I	144		HPLC				
3.6 (0.4)	Recommended							
$C_{11}H_{12}O_2$	2-Methylpropenoic acid, benzyl ester CAS # 2495-37-6							
2.16	I	144		HPLC				
2.7 (0.3)	Recommended							
$C_{12}H_{22}O_2$	2-Methylpropenoic acid, 2-ethylhexyl ester CAS # 688-84-6							
4.35	I	144		HPLC				
4.8 (0.5)	Recommended							
$C_{14}H_{26}O_2$	2-Methylpropenoic acid, isodecyl ester CAS # 29964-84-9							
4.92	I	144		HPLC				
5.9 (0.6)	Recommended							
$C_{11}H_{14}O_2$	3-Methylbutanoic acid, phenyl ester CAS # 15806-38-9							
3.18	D	220		SF	AS	W	AQ	46
3.18 (0.30)	Recommended							
$C_{14}H_{20}O_2$	3-Methylbutanoic acid, benzyl ester							
3.26	D	220		SF	AS	W	AQ	46
3.26 (0.30)	Recommended							
$C_8H_8O_2$	Benzoic acid, methyl ester CAS # 93-58-3							
2.14	D	221	21	SF	HPLC	W	AQ	
2.23	D	190	25	SF	AS	W	ORG	191
2.15	I	122		HPLC				
2.22	I	57		HPLC				
2.20 (0.15)	Recommended							

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{10}O_2$	Benzoic acid, ethyl ester				CAS # 93-89-0			
2.20	D	154		SF	AS			
*2.64	D	104						
2.64	D	221	21	SF	HPLC	W	AQ	
2.64[a]	?	222						
2.64	(0.20)	Recommended						
$C_{10}H_{12}O_2$	Benzoic acid, n-propyl ester				CAS # 2315-68-6			
1.80?	D	221	21	SF	HPLC	W	AQ	
3.18	(0.25)	Recommended						
$C_{10}H_{12}O_2$	Benzoic acid, isopropyl ester				CAS # 939-48-0			
3.09	I	122		HPLC				
*3.18	?	223						
3.18	(0.25)	Recommended						
$C_{11}H_{14}O_2$	Benzoic acid, n-butyl ester				CAS # 136-60-7			
3.74	I	122		HPLC				
3.74	(0.37)	Recommended						
$C_{12}H_{16}O_2$	Benzoic acid, isopentyl ester							
4.15	I	122		HPLC				
4.15	(0.40)	Recommended						
$C_{13}H_{10}O_2$	Benzoic acid, phenyl ester				CAS # 93-99-2			
3.58	D	104						
*3.59	D	104						
3.59	(0.25)	Recommended						
$C_{14}H_{12}O_2$	Benzoic acid, benzyl ester				CAS # 120-51-4			
*3.97	D	104						
3.97	(0.30)	Recommended						

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{13}H_{18}O_2$ 2-Ethyl-3-methylbutanoic acid, phenyl ester								
4.20	D	220		SF	AS	W	AQ	46
4.20 (0.40) Recommended								
$C_9H_{10}O_2$ Phenylethanoic acid, methyl ester CAS # 101-41-7								
*1.83	D	120		SF	AS	W	AQ	46
1.83 (0.20) Recommended								
$C_9H_{10}O_2$ 2-Methylbenzoic acid, methyl ester CAS # 89-71-4								
*2.75	D	104						
2.75 (0.25) Recommended								
$C_{10}H_{10}O_2$ 3-Phenylpropenoic acid, methyl ester (isomer not specified) CAS # 103-26-4								
*2.62	?	199						
2.62 (0.25) Recommended								
$C_{11}H_{12}O_2$ 3-Phenylpropenoic acid, ethyl ester (isomer not specified) CAS # 103-36-6								
2.91	D	154		SF	AS			
*2.99	?	199						
2.99 (0.25) Recommended								
$C_{18}H_{16}O_2$ 3-Phenylpropenoic acid, 3-phenylpropenyl ester CAS # 122-69-0								
*4.45	I	216		HPLC				
4.45 (0.40) Recommended								
$C_{10}H_{12}O_2$ 3-Phenylpropanoic acid, methyl ester CAS # 103-25-3								
*2.32	D	120		SF	AS	W	AQ	46
2.32 (0.20) Recommended								
$C_{10}H_{20}O_2$ Nonanoic acid, methyl ester CAS # 98-01-1								
4.32	D	9,10	25	G	GLC	W	Both	11
3.87 (0.40) Recommended								

Table 13. Esters (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{11}H_{18}O_2$	2,2-Dimethyl-3-(2-methylpropenyl)-cyclopropane carboxylic acid, methyl ester CAS # 24141-52-4							
*3.76	D	219	25	SF	AS	W	AQ	
3.76 (0.40) Recommended								
$C_{17}H_{22}O_2$	2,2-Dimethyl-3-(2-methylpropenyl)-cyclopropane carboxylic acid, benzyl ester CAS # 64312-78-3							
*5.49	D	219	25	SF	AS	W	AQ	
5.49 (0.50) Recommended								
$C_{11}H_{22}O_2$	Decanoic acid, methyl ester CAS # 110-42-9							
4.41	D	9,10	25	G	GLC	W	Both	11
4.41 (0.40) Recommended								
$C_{12}H_{16}O_2$	2-Phenyl-3-methylbutanoic acid, methyl ester							
3.33	D	220		SF	AS	W	AQ	46
3.33 (0.30) Recommended								

[a] D. E. Leahy and co-workers, personal communication.

Table 14. Halogenated compounds

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CCl_4	Tetrachloromethane			CAS # 56-23-5				
2.62	D	135	20	SF	GLC	W	Both	
2.73	D	108	23	SF	RC	W	Both	
*2.83	D	104					Both	
2.03	I	65		HPLC				
2.54	I	33	25	from water solubility correlation				
2.81	I	74	25	from UNIFAC activity coefficients				
2.83 (0.25) Recommended								
$CHCl_3$	Trichloromethane			CAS # 67-66-3				
1.90	D	108	23	SF	RC	W	Both	
1.94	D	104				D_2O		
*1.97	D	30,111		SF	GLC	W	one	46
1.43	I	33	25	from water solubility correlation				
1.91	I	74	25	from UNIFAC activity coefficients				
3.04?	I	65		HPLC				
1.97 (0.15) Recommended								
CH_2Cl_2	Dichloromethane			CAS # 75-09-2				
*1.25	D	104					Both	
1.25 (0.15) Recommended								
CH_2F_2	Difluoromethane			CAS # 75-10-5				
*0.20	D	104					Both	
0.20 (0.20) Recommended								
CH_2I_2	Diiodomethane			CAS # 75-11-6				
*2.30	D	104						
2.30 (0.20) Recommended								
CH_3Br	Bromomethane			CAS # 74-83-9				
*1.19	D	104						
1.19 (0.20) Recommended								

Table 14. Halogenated compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_3Cl		Chloromethane		CAS # 74-87-3				
*0.91	D	104					Both	
0.91	(0.20)	Recommended						
CH_3F		Fluoromethane		CAS # 593-53-3				
*0.51	D	104					Both	
0.51	(0.20)	Recommended						
CH_3I		Iodomethane		CAS # 74-88-4				
*1.51	D	104					Both	
1.69	D	147	19	SF		W	Both	148
1.51	(0.15)	Recommended						
C_2H_5Br		Bromoethane		CAS # 74-96-4				
*1.61	D	104					Both	
1.61	(0.20)	Recommended						
C_2H_5Cl		Chloroethane		CAS # 75-00-3				
*1.43	D	104					Both	
1.43	(0.20)	Recommended						
C_2H_5I		Iodoethane		CAS # 75-03-6				
*2.00	D	30,111		SF	GLC	W	AQ	46
2.00	(0.20)	Recommended						
C_3H_5Br		3-Bromo-1-propene		CAS # 106-95-6				
*1.79	D	9,10	25	G	HPLC	W	Both	11
1.79	(0.20)	Recommended						
C_3H_7Br		1-Bromopropane		CAS # 106-94-5				
*2.10	D	30,111		SF	GLC	W	one	46
2.10	(0.20)	Recommended						

Table 14. Halogenated compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_3H_7Cl		1-Chloropropane		CAS # 540-54-5				
*2.04	D	104					Both	
2.04	(0.20)	Recommended						
C_3H_7Cl		2-Chloropropane		CAS # 75-29-6				
*1.90	D	104						
1.90	(0.20)	Recommended						
C_4H_7Br		4-Bromo-1-butene		CAS # 5162-44-7				
2.53	D	9,10	25	G	HPLC	W	Both	11
2.34	(0.20)	Recommended						
C_4H_9Br		1-Bromobutane		CAS # 109-65-9				
*2.75	D	9,10	25	G	GLC	W	Both	11
2.75	D	58	25	G	HPLC	W	Both	11
2.64	I	58	25	from measured activity coefficients				
2.79	I	10	25	from measured activity coefficients				
2.75	(0.15)	Recommended						
C_4H_9Cl		1-Chlorobutane		CAS # 109-69-3				
2.39	D	30	25	SF	GLC	W	AQ	46
2.55	D	9,10	25	G	GLC	W	Both	11
*2.64	D	104					Both	
2.39	?	105						
2.64	(0.25)	Recommended						
C_4H_9F		1-Fluorobutane		CAS # 2366-52-1				
*2.58	D	104						
2.58	(0.30)	Recommended						

Table 14. Halogenated compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_5H_{11}Br$		1-Bromopentane		CAS # 110-53-2				
*3.37	D	9	25	G	GLC	W	Both	11
3.37	D	58	25	G	HPLC	W	Both	11
3.49	D	10	25	G	GLC	W	Both	
3.32	I	58	25	from measured activity coefficients				
3.37	(0.25)	Recommended						
$C_5H_{11}F$		1-Fluoropentane		CAS # 592-50-7				
*2.33	D	111		SF	GLC	W	AQ	46
2.05	I	33	25	from water solubility correlation				
2.33	(0.20)	Recommended						
C_6H_5Br		Bromobenzene		CAS # 108-86-1				
2.98	D	10	25	G	HPLC	W	Both	
*2.99	D	30,46	25	SF	AS	W	AQ	
3.01	D	114	25	SF	GLC	W	AQ	
2.84	I	33	25	from water solubility correlation				
2.94	I	116		HPLC				
3.02	I	92		HPLC				
3.02	I	122		HPLC				
3.15	I	65		HPLC				
2.99	(0.15)	Recommended						
C_6H_5Cl		Chlorobenzene		CAS # 108-90-7				
2.46	D	224	AMB	SF	AS	W	one	
2.60	D	108	23	SF	RC	W	Both	
2.81	D	10	25	G	HPLC	W	Both	
2.84	D	114	25	SF	GLC	W	AQ	
*2.84	D	30,46	25	SF	AS	W	AQ	
2.98	D	9,10	25	G	HPLC	W	Both	11
2.98	D	34	25	G	HPLC	W	Both	11
2.18?	?	150						
2.63	I	33	25	from water solubility correlation				
2.75[a]	I	64		HPLC				
2.83	I	10	25	from measured activity coefficients				
2.84	I	112		HPLC				
3.00	I	130		HPLC				
3.08	I	75	25	from UNIFAC activity coefficients				
2.84	(0.15)	Recommended						

Table 14. Halogenated compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_6H_5F		Fluorobenzene		CAS # 462-06-6				
*2.27	D	46	25	SF	AS	W	AQ	
2.27	(0.20)	Recommended						
C_6H_5I		Iodobenzene		CAS # 591-50-4				
*3.25	D	104						
3.28	D	9,10	25	G	HPLC	W	Both	11
3.03	I	33	25	from water solubility correlation				
3.37	I	65		HPLC				
3.25	(0.15)	Recommended						
$C_6H_{11}Br$		Bromocyclohexane		CAS # 108-85-0				
*3.20	D	139		SF	GLC	W		1
3.20	(0.25)	Recommended						
$C_6H_{13}Br$		1-Bromohexane		CAS # 111-25-1				
*3.80	D	9,10	25	G	GLC	W	Both	11
3.80	D	58	25	G	HPLC	W	Both	11
3.80	I	58	25	from measured activity coefficients				
3.80	(0.20)	Recommended						
C_7H_7Br		Benzyl bromide		CAS # 100-39-0				
*2.92	D	104						
2.92	(0.30)	Recommended						
C_7H_7Cl		Benzyl chloride		CAS # 100-44-7				
*2.30	D	225	22	SF	GLC,RC	W	Both	
2.30	(0.20)	Recommended						
C_7H_7Cl		2-Chlorotoluene		CAS # 95-49-8				
*3.42	D	104						
3.52	I	112		HPLC				
3.59	I	65		HPLC				
3.42	(0.20)	Recommended						

Table 14. Halogenated compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_7Cl	3-Chlorotoluene			CAS # 108-41-8				
*3.28	D	104						
3.28 (0.20) Recommended								
C_7H_7Cl	4-Chlorotoluene			CAS # 106-43-4				
*3.33	D	104						
3.30	?	131						
3.42	I	112		HPLC				
3.33 (0.15) Recommended								
$C_7H_{15}Br$	1-Bromoheptane			CAS # 629-04-9				
*4.36	D	9,10	25	G	GLC	W	Both	11
4.36	D	58	25	G	HPLC	W	Both	11
4.44	I	58	25	from measured activity coefficients				
4.36 (0.15) Recommended								
$C_7H_{15}Cl$	1-Chloroheptane			CAS # 629-06-1				
*4.15	D	9,10	25	G	GLC	W	Both	11
4.15 (0.25) Recommended								
$C_7H_{15}I$	1-Iodoheptane			CAS # 4282-40-0				
*4.70	D	9,10	25	G	GLC	W	Both	11
4.70 (0.30) Recommended								
$C_8H_{17}Br$	1-Bromooctane			CAS # 111-83-1				
*4.89	D	9,10	25	G	GLC	W	Both	11
4.89	D	58	25	G	HPLC	W	Both	11
5.09	I	58	25	from measured activity coefficients				
4.89 (0.35) Recommended								
$C_{10}H_7Cl$	1-Chloronaphthalene			CAS # 90-13-1				
3.90	D	226		SF	GLC	W	Both	68
3.90 (0.30) Recommended								

Table 14. Halogenated compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_7Cl$		2-Chloronaphthalene		CAS # 91-58-7				
3.98	D	226		SF	GLC	W	Both	68
4.07[b]	?	227						
3.98 (0.30) Recommended								
$C_{10}H_{21}Br$		1-Bromodecane		CAS # 112-29-8				
6.43	I	141		HPLC				
6.0 (0.5) Recommended								
$C_{12}H_9Cl$		2-Chlorobiphenyl		CAS # 2051-60-7				
*4.38	D	129	25	G	HPLC	W	Both	
4.50	D	34	25	G	GLC	W	Both	
4.59	D	68		SF	GLC	W	Both	
4.10	I	141		HPLC				
4.54[b]	?	228						
4.60	I	128		HPLC				
4.52 (0.30) Recommended								
$C_{12}H_9Cl$		3-Chlorobiphenyl		CAS # 2051-61-8				
*4.58	D	129	25	G	HPLC	W	Both	
4.71	D	68		SF	GLC	W	Both	
4.42	I	128		HPLC				
4.95[b]	?	228						
4.58 (0.30) Recommended								
$C_{12}H_9Cl$		4-Chlorobiphenyl		CAS # 2051-62-9				
4.49	D	129	25	G	HPLC	W	Both	
*4.61	D	68		SF	GLC	W	Both	
4.26[b]	?	227						
4.40	I	128		HPLC				
4.90[b]	?	229						
4.61 (0.30) Recommended								

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[a] Average value.

[b] From an unidentified literature source.

Table 15. Amines

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_5N	Aminomethane		CAS # 74-89-5		pK_a= 10.65			
*-0.57	D	147	20	SF	K	W	Both	148
-0.57	D	202	25	SF	RC	pH13		
-0.57	(0.10)	Recommended						
C_2H_7N	Aminoethane		CAS # 75-04-7		pK_a= 10.70			
-0.30^b	D	230	20	SF	T	W	AQ	
*-0.13	D	104				pH13		
-0.13	(0.10)	Recommended						
C_2H_7N	Dimethylamine		CAS # 124-40-3		pK_a= 10.77			
*-0.38	D	202	25	SF	RC	pH13		
-0.38	(0.10)	Recommended						
C_3H_7N	3-Amino-1-propene (allyl amine)				CAS # 107-11-9		pK_a= 9.51	
*0.03	D	104				pH13		
0.03	(0.10)	Recommended						
C_3H_9N	1-Aminopropane		CAS # 107-10-8		pK_a= 10.68			
0.28	D	230	20	SF	T	W	AQ	
*0.48	D	104				pH13		
0.48	(0.20)	Recommended						
C_3H_9N	2-Aminopropane		CAS # 75-31-0		pK_a= 10.63			
-0.03	D	104						
*0.26	D	104				pH13		
0.26	(0.15)	Recommended						
C_3H_9N	Methylethyl amine			CAS # 624-78-2		pK_a= 11 (est.)		
*0.15	D	104				pH13		
0.15	(0.10)	Recommended						

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_3H_9N	Trimethyl amine		CAS # 75-50-3		pK_a = 9.79			
*0.16	D	104					Both	
0.27	D	231	25	SF	T	W	Both	232
0.16 (0.10) Recommended								
C_4H_5N	Pyrrole		CAS # 109-97-7		pK_a = -4.1			
*0.75	D	111		SF	AS	W	one	46
0.75 (0.10) Recommended								
C_4H_9N	Pyrrolidine		CAS # 123-75-1		pK_a = 11.18			
*0.46	D	104				pH13		
0.46 (0.25) Recommended								
$C_4H_{11}N$	1-Aminobutane		CAS # 109-73-9		pK_a = 10.64			
-1.22^{a}	D	233	AMB	SF	RC	pH7	Both	3
0.68	D	147	20	SF	K	W	Both	148
0.80	D	92		SF				
0.81	D	104						
0.88	D	231	25	SF	T	W	Both	232
*0.97	D	104				pH13		
1.02^{b}	D	104				pH9.4		
0.86 (0.20) Recommended								
$C_4H_{11}N$	1-Amino-2-methylpropane (isobutyl amine)				CAS # 78-81-9		pK_a = 10.58	
*0.73	D	104				pH13		
0.88^{b}	D	104				pH9.4		
0.73 (0.15) Recommended								
$C_4H_{11}N$	2-Aminobutane (sec-butyl amine)			CAS # 513-49-5			pK_a = 10.56	
0.74	D	104				pH13		
0.74 (0.15) Recommended								
$C_4H_{11}N$	2-Methyl-2-aminopropane (tert-butyl amine)				CAS # 75-64-9			
*0.40	D	104					pK_a = 10.68	
0.40 (0.20) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_4H_{11}N$	Diethylamine			CAS # 109-89-7		pK_a = 11.07		
0.43	D	147	19	SF	K	W	Both	148
0.57	D	231	25	SF	T	W	Both	232
*0.58	D	104				pH13		
0.81	I	65		HPLC				
0.58	(0.15)	Recommended						
$C_4H_{11}N$	Ethyldimethyl amine			CAS # 598-56-1		pK_a = 10.16 (20°C)		
0.70	D	104						
0.70	(0.20)	Recommended						
C_5H_5N	Pyridine			CAS # 110-86-1		pK_a = 5.21		
0.62	D	115		SF	AS	pH7.4	AQ	
0.64	D	104						
*0.65	D	120		SF	AS	W	AQ	46
0.66	D	104						
0.68	D	104						
0.78[b]	D	235	25	SF	AS	NS	Both	
1.04	D	234		SF		W		124
0.54	I	75	25	from UNIFAC activity coefficients				
0.62	I	60		HPLC				
0.63	I	44	25	microelectrometric titration				
0.63	I	209	25	microelectrometric titration				
0.65	(0.05)	Recommended						
C_5H_7N	N-Methylpyrrole			CAS # 96-54-8		pK_a = -3.15		
*1.21	D	151		SF	HPLC	NS	Both	
1.21	D	104						
1.21	(0.20)	Recommended						
$C_5H_{11}N$	Allylethyl amine			CAS # 2424-02-4		pK_a = 10. (est.)		
*0.81	D	104				pH13		
0.81	(0.10)	Recommended						

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_5H_{11}N$		Piperidine	CAS # 110-89-4			pK_a= 11.13		
0.60^b	D	104				pH9.4		
*0.84	D	104				pH13		
0.85	D	104						
0.84 (0.10) Recommended								
$C_5H_{13}N$		1-Aminopentane	CAS # 110-58-7			pK_a= 10.61		
-0.86^a	D	233	AMB	SF	RC	pH7	Both	3
*1.49	D	104				pH13		
1.49^b	D	104				pH9.4		
1.49 (0.15) Recommended								
$C_5H_{13}N$		Methylbutyl amine	CAS # 110-68-9			pK_a= 11. (est.)		
*1.33	D	104						
1.33 (0.15) Recommended								
$C_5H_{13}N$		Ethylisopropyl amine	CAS # 19961-27-4			pK_a= 11. (est.)		
*0.93	D	104				pH13		
0.93 (0.10) Recommended								
C_6H_7N		Aniline	CAS # 62-53-3			pK_a= 4.60		
0.89	D	115		SF	AS	pH7.4	AQ	
0.89	D	171	25	SF	AS	pH5.6	AQ	
*0.90	D	30,46	25	SF	AS	W	AQ	
0.90	D	86	20	SF	AS	W	AQ	46
0.95^a	D	237	37	SF	AS	pH7.4	AQ	46
0.98	D	238		SF	AS	pH7.5	AQ	1
0.98	D	104						
0.85	?	150						
0.90^d	?	236						
0.91	I	112		HPLC				
0.93^e	I	64		HPLC				
0.95	I	166		HPLC				
0.99	I	75	25	from UNIFAC activity coefficients				
$1.02^{e,f}$	?	110						
1.08^g	I	65		HPLC				
1.08	I	93		HPLC				
1.09	I	92		HPLC				
0.90 (0.05) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_6H_7N	2-Methylpyridine			CAS # 109-06-8		pK_a= 5.95		
*1.11	D	104						
1.11 (0.15) Recommended								
C_6H_7N	3-Methylpyridine			CAS # 108-99-6		pK_a= 5.65		
*1.20	D	104						
1.19	I	98		HPLC				
1.20 (0.15) Recommended								
C_6H_7N	4-Methylpyridine			CAS # 108-89-4		pK_a= 6.02		
*1.22	D	104						
1.33[b]	D	235	25	SF	AS	NS	Both	
1.22 (0.10) Recommended								
$C_6H_{11}N$	Diallyl amine			CAS # 124-02-7		pK_a= 9.29		
*1.11	D	104				pH13		
1.11 (0.15) Recommended								
$C_6H_{13}N$	Aminocyclohexane			CAS # 108-91-8		pK_a= 10.67		
*1.49	D	104				pH13		
1.49 (0.10) Recommended								
$C_6H_{13}N$	Allylpropyl amine			CAS # 5666-21-7		pK_a= 10. (est.)		
*1.33	D	104				pH13		
1.33 (0.15) Recommended								
$C_6H_{13}N$	N-Methylpiperidine			CAS # 626-67-5		pK_a= 10.13		
-0.40[a]	D	239		SF		pH7.4		
*1.30	D	239		SF		pH11		
1.30 (0.15) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_6H_{15}N$	1-Aminohexane		CAS # 111-26-2		pK_a = 10.60			
-0.42[a]	D	233	AMB	SF	RC	pH7	Both	3
1.98	D	225	22	SF	GLC,RC	W	Both	
1.98[b]	D	104				pH9.4		
*2.06	D	104				pH13		
2.15	D	104				pH12		
2.11	?	240						
2.06 (0.10) Recommended								
$C_6H_{15}N$	Di-n-propylamine		CAS # 142-84-7			pK_a = 10.93		
1.46[b]	D	104				pH9.4		
*1.67	D	104				pH13		
1.73	D	104						
1.67 (0.08) Recommended								
$C_6H_{15}N$	Butyldimethyl amine		CAS # 927-62-8			pK_a = 10.19 (20°C)		
*1.70	D	104						
1.70 (0.20) Recommended								
$C_6H_{15}N$	Triethylamine		CAS # 121-44-8		pK_a = 10.76			
1.15[b]	D	104				pH9.4		
1.44	D	104						
1.45	D	104				pH13		
1.45 (0.10) Recommended								
C_7H_9N	Benzylamine		CAS # 100-46-9		pK_a = 9.36			
-1.39[a]	D	241	37	SF	RC	pH7	Both	
0.29[a]	D	241	37	SF	RC	pH9.9	Both	
1.03	D	179	20	SF	AS	pH >11	AQ	
*1.09	D	120		SF	AS	W	AQ	46
1.09 (0.10) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_9N	2-Methylaniline			CAS # 95-53-4		pK_a = 4.43		
1.29	D	242		SF	AS	W	AQ	46
*1.32	D	104						
1.42	D	238		SF	AS	pH7.5	AQ	1
1.34^{e}	I	64		HPLC				
1.40^{d}	?	236						
1.43	I	166		HPLC				
1.63	I	56		HPLC				
1.32 (0.10) Recommended								
C_7H_9N	3-Methylaniline			CAS # 108-44-1		pK_a = 4.70		
*1.40	D	46	25	SF	AS	W	AQ	
1.42	D	86	20	SF	AS	W	AQ	46
1.43	D	104						
1.45	I	166		HPLC				
1.40 (0.05) Recommended								
C_7H_9N	4-Methylaniline			CAS # 106-49-0		pK_a = 5.08		
1.39	D	238		SF	AS	pH7.5	AQ	1
*1.39	D	46	25	SF	AS	W	AQ	
1.40	D	86	20	SF	AS	W	AQ	46
1.41	D	104						
1.44	D	237	37	SF	AS	pH7.4	AQ	46
1.56	D	71	23	SF	AS		ORG	
1.39^{d}	?	236						
1.41^{e}	I	64		HPLC				
1.42	I	57		HPLC				
1.48	I	166		HPLC				
1.39 (0.05) Recommended								
C_7H_9N	N-Methylaniline			CAS # 100-61-8		pK_a = 4.85		
*1.66	D	104						
1.82	D	242		SF	AS	W	AQ	46
1.66^{d}	?	236						
1.68	?	223						
1.70	I	57		HPLC				
1.66 (0.15) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_7H_9N 2-Ethylpyridine CAS # 100-71-0 $pK_a = 5.93$								
*1.69[a]	D	189	25	SF	AS	pH7	AQ	46
1.69 (0.15) Recommended								
C_7H_9N 2,6-Dimethylpyridine CAS # 108-48-5 $pK_a = 6.67$								
*1.68[a]	D	189	25	SF	AS	pH7	AQ	46
1.63	I	57		HPLC				
1.68 (0.15) Recommended								
$C_7H_{13}N$ 1-Azabicyclo 2,2,2 octane (quinuclidine) CAS # 100-76-5 $pK_a = 10.95$								
1.20[a]	D	104				pH9.4		
*1.38	D	104				pH13		
1.38 (0.15) Recommended								
$C_7H_{15}N$ N-Ethylpiperidine CAS # 766-09-6 $pK_a = 10.45$								
-1.52[b]	D	239		SF		pH7.4		
1.30?	D	239		SF		pH11		
1.88 (0.25) Recommended								
$C_7H_{17}N$ 1-Aminoheptane CAS # 111-68-2 $pK_a = 10.66$								
0.15[a]	D	233	AMB	SF	RC	pH7	Both	3
*2.57[b]	D	104				pH9.4		
2.57 (0.25) Recommended								
$C_7H_{17}N$ 2-Aminoheptane CAS # 44652-67-7 $pK_a = 10.58$								
*2.40	D	243		SF	GLC	pH13	AQ	
2.40 (0.20) Recommended								
$C_7H_{17}N$ Propyl-n-butyl amine CAS # 20193-21-9 $pK_a = 11.$ (est.)								
*2.12	D	104				pH13		
2.12 (0.20) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_7H_{17}N$	Propylisobutyl amine			CAS # 39190-66-4		$pK_a = 11.$ (est.)		
*2.07	D	104				pH13		
2.07 (0.20) Recommended								
$C_7H_{17}N$	Propyl-sec-butyl amine			CAS # 39190-67-5		$pK_a = 11.$ (est.)		
*1.91	D	104				pH13		
1.91 (0.20) Recommended								
C_8H_7N	Indole		CAS # 120-72-9		$pK_a = -3.17$			
2.00	D	104						
2.12	D	104						
*2.14	D	111		SF	AS	W	one	46
2.25	D	40	25	SF	AS	pH7.4	Both	117
1.66	I	56		HPLC				
1.81	I	65		HPLC				
1.92	I	92		HPLC				
2.14 (0.10) Recommended								
C_8H_9N	N-Benzylidenemethyl amine			CAS # 622-29-7				
*1.64	D	104						
1.64 (0.15) Recommended								
$C_8H_{11}N$	1-Amino-2-phenylethane			CAS # 64-04-0		$pK_a = 9.82$		
-1.39[a]	D	241	37	SF	RC	pH7	Both	
-1.18[a]	D	246	AMB	SF	RC	pH7.4	Both	
-1.14[a]	D	245		SF	FLorRC	pH7.4	AQ	
0.35[a]	D	241	37	SF	RC	pH10	Both	
1.16[b]	D	246	AMB	SF	RC	pH7.4	Both	
1.28	D	247	25	SF	AS		AQ	
1.37[b]	D	179	20	SF	AS		AQ	
1.38	D	245		SF	FLorRC	pH7.4	AQ	
*1.41	D	120		SF	AS	W	AQ	46
1.52[b]	D	244	AMB	SF	AS	pH8	AQ	46,248
1.41 (0.05) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{11}N$ 2-Ethylaniline CAS # 578-54-1 pK_a= 4.34								
*1.74	D	104						
1.74 (0.25) Recommended								
$C_8H_{11}N$ 4-Ethylaniline CAS # 589-16-2 pK_a= 5.00								
*1.96[a]	D	237	37	SF	AS	pH7.4	AQ	46
1.97	D	238		SF	AS	pH7.5	AQ	1
1.96 (0.10) Recommended								
$C_8H_{11}N$ 2,4-Dimethylaniline CAS # 95-68-1 pK_a= 4.87								
1.68	D	238		SF	AS	pH7.5	AQ	1
1.68 (0.20) Recommended								
$C_8H_{11}N$ N-Methylbenzyl amine CAS # 103-67-3 pK_a= 9.56								
*1.52	D	104				pH13		
1.52 (0.20) Recommended								
$C_8H_{11}N$ N-Ethylaniline CAS # 103-69-5 pK_a= 5.12								
2.26	D	242	25	SF	AS	W	AQ	46
*2.16[d]	?	236						
2.16 (0.20) Recommended								
$C_8H_{11}N$ 2,N-Dimethylaniline CAS # 611-21-2 pK_a= 4.60								
*2.16[d]	?	236						
2.16 (0.20) Recommended								
$C_8H_{11}N$ 4,N-Dimethylaniline CAS # 623-08-5 pK_a= 5.25								
*2.15[d]	?	236						
2.15 (0.20) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_8H_{11}N$	N,N-Dimethylaniline			CAS # 121-69-7		$pK_a = 5.10$		
2.29	D	154		SF	AS			
*2.31	D	46	25	SF	AS	W	AQ	
2.62	D	40	25	SF	AS	pH7.4	Both	117
2.31^d	?	236						
2.31 (0.10) Recommended								
$C_8H_{11}N$	4-n-Propylpyridine			CAS # 1122-81-2		$pK_a = 6.05$		
*2.10	D	104						
2.10 (0.20) Recommended								
$C_8H_{11}N$	2,4,6-Trimethylpyridine			CAS # 108-75-8		$pK_a = 7.42$		
*1.88	D	104						
2.01	D	98	23	SF	AS	W	Both	143
1.88 (0.25) Recommended								
$C_8H_{19}N$	1-Aminooctane			CAS # 111-86-4		$pK_a = 10.61$		
0.76^a	D	233	AMB	SF	RC	pH7	Both	3
3.09 (0.40) Recommended								
$C_8H_{19}N$	1-Amino-2-ethylhexane			CAS # 104-75-6		$pK_a = 11.$ (est.)		
*2.82^b	D	104				pH9.4		
2.82 (0.35) Recommended								
$C_8H_{19}N$	Di-n-butylamine			CAS # 111-92-2		$pK_a = 11.25$		
2.68	D	104						
*2.83	D	104				pH9.4		
2.83 (0.30) Recommended								
$C_8H_{19}N$	Ethyldi-n-propyl amine			CAS # 20634-92-8		$pK_a = 11.$ (est.)		
*2.68	D	104						
2.68 (0.30) Recommended								

Table 15 . Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_9H_7N		Quinoline	CAS # 91-22-5		pK_a = 4.87			
*2.03	D	120		SF	AS	W	AQ	46
2.06	D	40	25	SF	AS	pH7.4	Both	117
1.88	I	57		HPLC				
2.02	I	60		HPLC				
2.03[d]	?	236						
2.03	(0.10)	Recommended						
C_9H_7N		Isoquinoline	CAS # 119-65-3		pK_a = 5.39			
*2.08	D	111		SF	AS	W	one	46
2.08	(0.20)	Recommended						
C_9H_9N		1-Methylindole	CAS # 603-76-9		pK_a = -2.14			
*2.72	D	104						
2.72	(0.25)	Recommended						
C_9H_9N		2-Methylindole	CAS # 95-20-5		pK_a = -0.19			
*2.53[a]	D	249	25	SF	AS	pH7.4	Both	
2.53	(0.25)	Recommended						
C_9H_9N		3-Methylindole	CAS # 83-34-1		pK_a = -3.40			
*2.60	D	40	25	SF	AS	pH7.4	Both	117
2.60	(0.25)	Recommended						
C_9H_9N		5-Methylindole	CAS # 614-96-0		pK_a = -3.3			
*2.68	D	40	25	SF	AS	pH7.4	Both	117
2.68	(0.25)	Recommended						
$C_9H_{11}N$		cis-1-Amino-2-phenylcyclopropane			CAS # 69684-88-4		pK_a = 10. (est.)	
*1.49	D	243		SF	GLC	pH13		
1.49	(0.20)	Recommended						

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{11}N$ trans-1-Amino-2-phenylcyclopropane CAS # 95-62-5 pK_a= 10. (est.)								
*1.58	D	243		SF	GLC	pH13		
1.58 (0.20) Recommended								
$C_9H_{11}N$ 1,2,3,4-Tetrahydroquinoline CAS # 635-46-1 pK_a= 5.03								
*2.29[d]	?	236						
2.29 (0.25) Recommended								
$C_9H_{13}N$ 1-Amino-3-phenylpropane CAS # 2038-57-5 pK_a= 10. (est.)								
*1.83	D	120		SF	AS	W	AQ	46
1.83	D	179	20	SF	AS	pH>12	AQ	
1.83 (0.20) Recommended								
$C_9H_{13}N$ 1-Phenyl-2-aminopropane (amphetamine) CAS # 300-62-9 pK_a= 9.90								
-1.18	D	104				pH1		
-0.94[a]	D	246	AMB	SF	RC	pH7.4	Both	
-0.84[a]	D	245		SF	FLorRC	pH7.4	AQ	
0.31[a]	D	251	25	SF	RC	pH7.4	Both	3
1.54[b]	D	246	AMB	SF	RC	pH7.4	Both	
1.56	D	104				pH10.2		
1.64[b]	D	245		SF	FLorRC	pH7.4	AQ	
1.69	D	247	25	SF	AS	c	AQ	
*1.76	D	104						
1.81	D	243		SF	GLC	pH13	AQ	
2.05[b]	D	121	25	SF	RC	pH7.4	Both	3
-0.68	?	250				pH7.2		
1.76 (0.10) Recommended								
$C_9H_{13}N$ 4-n-Propylaniline CAS # 622-80-0 pK_a= 4.9 (est.)								
2.40	D	238		SF	AS	pH7.5	AQ	1
2.40 (0.25) Recommended								
$C_9H_{13}N$ 4-Isopropylaniline CAS # 99-88-7 pK_a= 4.85 (20°C)								
*2.23[a]	D	237	37	SF	AS	pH7.4	AQ	46
2.31	D	238		SF	AS	pH7.5	AQ	1
*2.49[a]	D	237	37	SF	AS	pH7.4	AQ	46
2.34 (0.25) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{13}N$ N-Propylaniline CAS # 622-80-0 $pK_a = 4.92$								
*2.45	D	242		SF	AS	W	AQ	46
2.45 (0.25) Recommended								
$C_9H_{13}N$ 2-tert-Butylpyridine CAS # 5944-41-2 $pK_a = 5.83$								
*2.40	I	98		HPLC				143
2.40 (0.25) Recommended								
$C_9H_{13}N$ 4-n-Butylpyridine CAS # 5335-75-1 $pK_a = 6.0$ (est.)								
3.13^b	D	252	25	SF	AS	NS	AQ	
3.13 (0.30) Recommended								
$C_9H_{13}N$ N,N-Dimethylbenzyl amine CAS # 103-83-3 $pK_a = 8.97$								
1.79^b	D	104				pH8		
1.80^b	D	104				pH9.4		
1.91	D	104						
*1.98	D	104				pH13		
1.98 (0.25) Recommended								
$C_9H_{13}N$ 2,N,N-Trimethylaniline CAS # 609-72-3 $pK_a = 5.98$								
*2.85	D	192	AMB	SF	AS	pH>8	AQ	
2.81^d	?	236						
2.85 (0.25) Recommended								
$C_9H_{13}N$ 3,N,N-Trimethylaniline CAS # 121-72-2 $pK_a = 5.27$								
*2.80	D	192	AMB	SF	AS	pH>7	AQ	
2.80 (0.25) Recommended								
$C_9H_{13}N$ 4,N,N-Trimethylaniline CAS # 99-97-8 $pK_a = 5.19$								
2.61	D	192	AMB	SF	AS	pH>7	AQ	
$*2.81^d$	?	236						
2.81 (0.30) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_9H_{15}N$	Triallyl amine			CAS # 102-70-5		$pK_a = 8.31$		
*2.59	D	104				pH13		
2.59 (0.25) Recommended								
$C_9H_{19}N$	2-Amino-3-cyclohexylpropane			CAS # 54704-34-6			$pK_a = 11.$ (est.)	
*2.96	D	243		SF	GLC	pH13	AQ	
2.96 (0.30) Recommended								
$C_9H_{21}N$	1-Aminononane			CAS # 112-20-9		$pK_a = 10.64$		
1.33^a	D	233	AMB	SF	RC	pH7	Both	3
3.60 (0.35) Recommended								
$C_9H_{21}N$	Tri-n-propyl amine			CAS # 102-69-2		$pK_a = 10.46$		
2.79	D	104						
*2.79^b	D	104				pH9.4		
2.79 (0.30) Recommended								
$C_{10}H_9N$	1-Aminonaphthalene			CAS # 134-32-7		$pK_a = 3.92$		
2.27	D	238		SF	AS	pH7.5	AQ	1
2.25^d	?	236						
2.25 (0.25) Recommended								
$C_{10}H_9N$	2-Aminonaphthalene			CAS # 91-59-8		$pK_a = 4.15$		
2.40	D	238		SF	AS	pH7.5	AQ	1
2.40	I	75	25	from UNIFAC activity coefficients				
2.40 (0.25) Recommended								
$C_{10}H_9N$	2-Phenylpyrrole			CAS # 3042-22-6		$pK_a = -4.5$ (est.)		
2.76	I	143		HPLC				
2.76 (0.30) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_{11}N$ 1,2-Dimethylindole CAS # 875-79-6 pK_a= -0.1 (est.)								
*2.82	D	40	25	SF	AS	pH7.4	Both	117
2.82 (0.30) Recommended								
$C_{10}H_{13}N$ 2-Amino-1,2,3,4-tetrahydronaphthalene CAS # 2954-50-9 pK_a= 11. (est.)								
*2.08	D	243		SF	GLC	pH13	AQ	
2.08 (0.20) Recommended								
$C_{10}H_{13}N$ 2-Phenylpyrrolidine CAS # 1006-64-0 pK_a= 9.60								
1.89	I	143	23	microelectrometric titration				
1.89 (0.20) Recommended								
$C_{10}H_{13}N$ 3-Methyl-1,2,3,4-tetrahydroisoquinoline CAS # 29726-60-1 pK_a= 5.6 (est.)								
*1.93	D	243		SF	GLC	pH13	AQ	
1.93 (0.20) Recommended								
$C_{10}H_{15}N$ 1-Amino-4-phenylbutane CAS # 13214-66-9 pK_a= 10.36								
-0.67^a	D	253		SF	AS	pH6.8	AQ	
*2.40	D	179	20	SF	AS	pH>12	AQ	
2.45	D	243		SF	GLC	pH13	AQ	
2.40 (0.15) Recommended								
$C_{10}H_{15}N$ 1-Phenyl-2-aminobutane CAS # 53309-89-0 pK_a= 10. (est.)								
*2.28	D	247	25	SF	AS	c	AQ	
2.28 (0.20) Recommended								
$C_{10}H_{15}N$ 4-n-Butylaniline CAS # 104-13-2 pK_a= 4.8 (est.)								
3.05	D	238		SF	AS	pH7.5	AQ	1
3.05 (0.30) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{10}H_{15}N$		4-tert-Butylaniline		CAS # 769-92-6		pK_a= 4.95		
2.47	D	238		SF	AS	pH7.5	AQ	1
2.47 (0.25) Recommended								
$C_{10}H_{15}N$		2,6-Diethylaniline		CAS # 579-66-8		pK_a= 4.0 (est.)		
0.95?	?	150						
3.1 (0.3) Recommended								
$C_{10}H_{15}N$		N-Butylaniline		CAS # 1126-78-9		pK_a= 5.28		
3.58	D	242		SF	AS	W	AQ	46
3.10 (0.20) Recommended								
$C_{10}H_{15}N$		N-Methyl-2-amino-3-phenylpropane (methamphetamine)					CAS # 537-46-2	
-1.30	D	104				pH1	pK_a= 11. (est.)	
-1.18	D	104				pH1		
*2.07	D	104				pH13		
2.16	D	243		SF	GLC	pH13	AQ	
2.07 (0.20) Recommended								
$C_{10}H_{15}N$		4-Pentylpyridine		CAS # 2961-50-4		pK_a= 6.0 (est.)		
3.75^b	D	252	25	SF	AS	NS	AQ	
3.45 (0.30) Recommended								
$C_{10}H_{15}N$		N,N-Diethylaniline		CAS # 91-66-7		pK_a= 6.55		
*3.31^d	?	236						
3.31 (0.20) Recommended								
$C_{10}H_{23}N$		1-Aminodecane		CAS # 2016-57-1		pK_a= 10.64		
1.92^a	D	233	AMB	SF	RC	pH7	Both	3
4.1 (0.4) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{11}H_9N$	2-Phenylpyridine			CAS # 1008-89-5		pK_a= 4.63		
*2.63	D	104					Both	
2.68	I	143		HPLC				
2.63	(0.25)	Recommended						
$C_{11}H_9N$	4-Phenylpyridine			CAS # 939-23-1		pK_a= 5.45		
2.45	D	104						
*2.59	D	104						
2.62	D	104					Both	
2.58	I	143		HPLC				
2.59	(0.10)	Recommended						
$C_{11}H_{13}N$	2-Endoamino-benzobicyclo [2,2,1] -heptane					CAS # 58742-04-4	pK_a= 11. (est.)	
*2.00	D	254		SF	GLC	pH13	Both	
2.00	(0.20)	Recommended						
$C_{11}H_{13}N$	2-Exoamino-benzobicyclo [2,2,1] -heptane					CAS # 62624-26-4	pK_a= 11. (est.)	
*2.09	D	254		SF	GLC	pH13	Both	
2.09	(0.20)	Recommended						
$C_{11}H_{13}N$	9-Endoamino-benzobicyclo [2,2,1] -heptane					CAS # 72597-35-4	pK_a= 11. (est.)	
*2.08	D	254		SF	GLC	pH13	Both	
2.08	(0.20)	Recommended						
$C_{11}H_{13}N$	9-Exoamino-benzobicyclo [2,2,1] -heptane					CAS # 14098-20-5	pK_a= 11. (est.)	
*2.13	D	254		SF	GLC	pH13	Both	
2.13	D	243		SF	GLC	pH13	AQ	
2.13	(0.20)	Recommended						

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{11}H_{15}N$ N-Methyl-2-amino-1,2,3,4-tetrahydronaphthalene CAS # 19485-85-9 pK_a= 10. (est.)								
*2.38	D	243		SF	GLC	pH13	AQ	
2.38 (0.20) Recommended								
$C_{11}H_{15}N$ 4-Phenylpiperidine CAS # 771-99-3 pK_a= 10.41								
2.39	I	143	23	microelectrometric titration				
2.39 (0.20) Recommended								
$C_{11}H_{15}N$ N-Phenylpiperidine CAS # 4096-20-2 pK_a= 7.0 (est.)								
2.78	D	104						
*2.98	D	104				pH13		
2.98 (0.30) Recommended								
$C_{11}H_{17}N$ 1-Phenyl-2-aminopentane CAS # 63951-01-9 pK_a= 10.03								
*2.79	D	247	25	SF	AS	pH>12	AQ	
2.79 (0.25) Recommended								
$C_{11}H_{17}N$ 1-Phenyl-2-amino-3-methylbutane CAS # 46114-16-3 pK_a= 9.90								
*2.59	D	247	25	SF	AS	pH>12	AQ	
2.59 (0.25) Recommended								
$C_{11}H_{17}N$ 1-(N-Methylamino)-4-phenylbutane CAS # 4265-99-0 pK_a= 11. (est.)								
2.76	D	243		SF	GLC	pH13	AQ	
2.76 (0.25) Recommended								
$C_{11}H_{17}N$ 1-(N,N-Dimethylamino)-3-phenylpropane CAS # 1199-99-1 pK_a= 10. (est.)								
*2.73	D	120		SF	AS	W	AQ	46
2.73 (0.27) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{11}H_{17}N$	4-Hexylpyridine			CAS # 27876-24-0		$pK_a = 6.0$ (est.)		
4.35[b]	D	252	25	SF	AS	NS	AQ	
4.35 (0.40) Recommended								
$C_{11}H_{23}N$	1-cyclooctyl-2-aminopropane				$pK_a = 11.$ (est.)			
*3.70	D	243		SF	GLC	pH13	AQ	
3.70 (0.30) Recommended								
$C_{12}H_9N$	Carbazole		CAS # 86-74-8		$pK_a = -4.$ (est.)			
3.29	D	40	25	SF	AS	pH7.4	Both	117
*3.72	D	104						
3.76	D	104						
3.01	I	65		HPLC				
3.72 (0.40) Recommended								
$C_{12}H_{11}N$	2-Aminobiphenyl			CAS # 90-41-5		$pK_a = 3.82$ (22°C)		
2.83[a]	D	104				pH7.4		
*2.84	D	104						
2.84 (0.25) Recommended								
$C_{12}H_{11}N$	4-Aminobiphenyl			CAS # 92-67-1		$pK_a = 4.26$		
2.86	D	238		SF	AS	pH7.5	AQ	1
2.86 (0.25) Recommended								
$C_{12}H_{11}N$	Diphenylamine			CAS # 122-39-4		$pK_a = 0.78$		
3.22	D	40	25	SF	AS	pH7.4	Both	117
3.34	D	104						
3.37	D	92		SF				
3.42	D	86	20	SF	AS	W	AQ	46
*3.50	D	104						
2.37?	I	56		HPLC				
2.69?[e]	I	64		HPLC				
3.50 (0.25) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{12}H_{15}N$	2-Endoamino-benzobicyclo[2,2,2]-octane					CAS # 14342-36-0		
							pK_a = 11. (est.)	
*2.29	D	254		SF	GLC	pH13	Both	
2.29 (0.20) Recommended								
$C_{12}H_{15}N$	2-Exoamino-benzobicyclo[2,2,2]-octane					CAS # 15537-20-9		
							pK_a = 11. (cst.)	
*2.32	D	254		SF	GLC	pH13	Both	
2.32 (0.20) Recommended								
$C_{12}H_{15}N$	2-Endomethylamino-benzobicyclo[2,2,1]-heptane					CAS # 58742-05-5		
							pK_a = 11. (est.)	
*2.32	D	254		SF	GLC	pH13	Both	
2.32 (0.20) Recommended								
$C_{12}H_{15}N$	2-Exomethylamino-benzobicyclo[2,2,1]-heptane					CAS # 62624-27-5		
							pK_a = 11. (est.)	
*2.41	D	254		SF	GLC	pH13	Both	
2.41 (0.20) Recommended								
$C_{12}H_{15}N$	9-Endomethylamino-benzobicyclo[2,2,1]-heptane					CAS # 86992-69-0		
							pK_a = 11. (est.)	
*2.37	D	254		SF	GLC	pH13	Both	
2.37 (0.20) Recommended								
$C_{12}H_{15}N$	9-Exomethylamino-benzobicyclo[2,2,1]-heptane					CAS # 86943-79-5		
							pK_a = 11. (est.)	
*2.47	D	254		SF	GLC	pH13	Both	
2.47	D	243		SF	GLC	pH13	AQ	
2.47 (0.25) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{12}H_{17}N$		4-Cyclohexylaniline		CAS # 6373-50-8		$pK_a = 4.96$		
3.31	D	238		SF	AS	pH7.5	AQ	1
*3.65	D	104						
3.65 (0.30) Recommended								
$C_{12}H_{19}N$		1-Phenyl-2-aminohexane		CAS # 67309-36-8		$pK_a = 10.04$		
*3.36	D	247	25	SF	AS	pH>12	AQ	
3.36 (0.20) Recommended								
$C_{12}H_{19}N$		1-Phenyl-2-amino-4-methylpentane			CAS # 67309-38-0			
						$pK_a = 10.03$		
*3.29	D	247	25	SF	AS	pH>12	AQ	
3.29 (0.30) Recommended								
$C_{12}H_{19}N$		1-Phenyl-2-amino-3,3-dimethylbutane			CAS # 67309-37-9			
						$pK_a = 9.64$		
*2.91	D	247	25	SF	AS	pH>12	AQ	
2.91 (0.30) Recommended								
$C_{12}H_{19}N$		1-(3,4,5-Trimethylphenyl)-2-aminopropane				$pK_a = 10.$ (est.)		
1.48?[b]	D	248	AMB	SF	AS	pH7.4	AQ	
3.50 (0.35) Recommended								
$C_{12}H_{19}N$		2,6-Diisopropylaniline		CAS # 24544-04-5		$pK_a = 4.0$ (est.)		
*3.18	D	104						
3.18 (0.30) Recommended								
$C_{12}H_{19}N$		4-Heptylpyridine		CAS # 40089-90-5		$pK_a = 6.0$ (est.)		
5.00[b]	D	252	25	SF	AS	NS	AQ	
5.00 (0.50) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{13}H_9N$ Acridine CAS # 260-94-6 $pK_a = 10.65$								
3.29^a	D	255		SF	AS	pH7.4		
3.32	D	132		SF	GLC	pH7	Both	
*3.40	?	124						
3.62	?	198						
3.40 (0.25) Recommended								
$C_{13}H_{13}N$ N-Benzylaniline CAS # 103-32-2 $pK_a = 4.04$								
*3.13	D	104						
3.13 (0.30) Recommended								
$C_{13}H_{13}N$ N,N-Diphenylaminomethane CAS # 552-82-9 $pK_a = 0.7$ (est.)								
3.16	D	104						
*3.90	D	104				pH13		
3.90 (0.30) Recommended								
$C_{14}H_{11}N$ 2-Aminoanthracene CAS # 613-13-8 $pK_a = 4.1$								
4.13?	D	217	AMB	SF	RC	W	Both	134
3.4 (0.3) Recommended								
$C_{15}H_{11}N$ 2-Phenylquinoline CAS # 612-96-4 $pK_a = 4.4$ (est.)								
*3.90	D	104						
3.96	D	104						
4.14^a	D	104				pH7.4		
3.90 (0.40) Recommended								
$C_{15}H_{17}N$ 1,3-Diphenyl-2-aminopropane CAS # 4275-43-8 $pK_a = 9.31$								
*3.35	D	247	25	SF	AS	pH>12	AQ	
3.35 (0.35) Recommended								
$C_{16}H_{13}N$ N-Phenyl-1-aminonaphthalene CAS # 90-30-2 $pK_a = 0.8$ (est.)								
4.20	D	256	22	SF	FL	W	Both	
4.20 (0.40) Recommended								

Table 15. Amines (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_{16}H_{19}N$ 1-Amino-4,4-diphenylbutane pK_a= 9.0 (est.)								
0.74[a]	D	253		SF	AS	pH6.8	AQ	1
4.0 (0.4) Recommended								
$C_{18}H_{13}N$ 6-Aminochrysene CAS # 2642-98-0 pK_a= 3.7 (est.)								
*4.98	D	217	AMB	SF	RC	W	Both	134
4.98 (0.50) Recommended								
$C_{18}H_{15}N$ Triphenylamine CAS # 603-34-9 pK_a= -5 (est.)								
5.70	D	132		SF	GLC	pH7	Both	
*5.74	D	104						
5.74 (0.50) Recommended								
$C_{18}H_{23}N$ N,N-Dimethyl-1-amino-4,4-diphenylbutane pK_a= 10. (est.)								
2.30[a]	D	253		SF	AS	pH6.8	AQ	1
4.8 (0.5) Recommended								

[a] Not ion-corrected.

[b] Ion-corrected.

[c] Buffer, pH not specified.

[d] From an unidentified literature source.

[e] Average value.

[f] D. Kotzias, personal communication.

[g] From a restricted correlation plot.

Table 16. Nitriles

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_2H_3N	Ethanenitrile	CAS # 75-05-8						
-0.54	D	257	AMB	SF	GLC	W	AQ	194
*-0.34	D	111		SF	GLC	W	AQ	46
-0.34	(0.05) Recommended							
C_3H_3N	Propenenitrile (acrylonitrile)	CAS # 107-13-1						
0.00	D	218		SF				
0.09	D	257	AMB	SF	GLC	W	AQ	194
*0.25	D	151		SF	HPLC	NS	Both	
0.25	(0.20) Recommended							
C_3H_5N	Propanenitrile	CAS # 107-12-0						
-0.10	D	257	AMB	SF	GLC	W	AQ	194
0.04	D	147	18	SF	K	W	Both	148
*0.16	D	30,111		SF	GLC	W	AQ	46
0.16	(0.05) Recommended							
C_4H_5N	3-Butenenitrile (allylnitrile)	CAS # 109-75-1						
*0.40	D	257	AMB	SF	GLC	W	AQ	194
0.40	(0.10) Recommended							
C_4H_5N	2-Methylpropenenitrile (methacrylonitrile)	CAS # 126-98-7						
*0.68	D	257	AMB	SF	GLC	W	AQ	194
0.68	(0.25) Recommended							
C_4H_7N	Butanenitrile	CAS # 109-74-0						
0.53	D	257	AMB	SF	GLC	W	AQ	194
0.60	(0.10) Recommended							
C_4H_7N	Methylpropanenitrile	CAS # 78-82-0						
*0.46	D	257	AMB	SF	GLC	W	AQ	194
0.46	(0.25) Recommended							

Table 16. Nitriles (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_5H_9N Pentanenitrile CAS # 110-59-8								
*0.94	D	257	AMB	SF	GLC	W	AQ	194
0.94	(0.30) Recommended							
C_5H_9N 2-Methylbutanenitrile CAS # 18936-17-9								
*1.05	D	257	AMB	SF	GLC	W	AQ	194
1.05	(0.10) Recommended							
C_5H_9N 3-Methylbutanenitrile CAS # 625-28-5								
*0.85	D	257	AMB	SF	GLC	W	AQ	194
0.85	(0.35) Recommended							
$C_6H_{11}N$ Hexanenitrile CAS # 628-73-9								
*1.66	D	257	AMB	SF	GLC	W	AQ	194
1.66	(0.20) Recommended							
$C_6H_{11}N$ 4-Methylpentanenitrile CAS # 542-54-1								
*1.54	D	257	AMB	SF	GLC	W	AQ	194
1.54	(0.15) Recommended							
C_7H_5N Benzonitrile CAS # 100-47-0								
*1.56	D	46	25	SF	AS	W	AQ	
1.56	D	190	25	SF	AS	W	ORG	191
1.56	D	257	AMB	SF	GLC	W	AQ	194
1.50	I	57		HPLC				
1.57	?	131						
1.56	(0.05) Recommended							
C_8H_7N Phenylethanenitrile CAS # 140-29-4								
*1.56	D	120		SF	AS	W	AQ	46
1.61	D	257	AMB	SF	GLC	W	AQ	194
1.44	I	57		HPLC				
1.47[a]	I	64		HPLC				
1.56	(0.20) Recommended							

Table 16. Nitriles (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_8H_7N	2-Methylbenzonitrile			CAS # 529-19-1				
*2.21	D	104						
2.21 (0.20) Recommended								
$C_8H_{15}N$	Octanenitrile		CAS # 124-12-9					
*2.75	D	257	AMB	SF	GLC	W	AQ	194
2.75 (0.25) Recommended								
C_9H_7N	3-Phenylpropenenitrile (cinnamonitrile, isomer not specified)							
1.94	I	57		HPLC		CAS # 1885-38-7		
*1.96	?	199						
1.94 (0.20) Recommended								
C_9H_9N	Benzylethanenitrile			CAS # 645-59-0				
1.66	D	104						
1.70	D	257	AMB	SF	GLC	W	AQ	194
*1.72	D	120		SF	AS	W	AQ	46
1.70	?	199						
1.72 (0.15) Recommended								
C_9H_9N	4-Methylphenylethanenitrile				CAS # 2947-61-7			
1.62	?	131						
1.8 (0.2) Recommended								

[a] Average value.

Table 17. Nitro compounds

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_3NO_2		Nitromethane		CAS # 75-52-5				
*-0.35	D	104					Both	
-0.33	D	111		SF	AS	W	one	46
0.08	D	147	20	SF	K	W	Both	148
-0.33	(0.05)	Recommended						
$C_2H_5NO_2$		Nitroethane		CAS # 79-24-3				
0.18	D	111		SF	AS	W	one	46
*0.18	D	104					Both	
0.18	(0.10)	Recommended						
$C_3H_7NO_2$		1-Nitropropane		CAS # 108-03-2				
*0.87	D	104					Both	
0.87	(0.07)	Recommended						
$C_4H_9NO_2$		1-Nitrobutane		CAS # 627-05-4				
*1.47	D	104					Both	
1.47	(0.12)	Recommended						
$C_4H_9NO_2$		2-Methyl-2-nitropropane		CAS # 594-70-7				
1.01	D	104						
*1.17	D	104						
1.17	(0.15)	Recommended						
$C_5H_{11}NO_2$		1-Nitropentane		CAS # 628-05-7				
*2.01	D	104					Both	
2.01	(0.20)	Recommended						

Table 17. Nitro compounds (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_6H_5NO_2$		Nitrobenzene		CAS # 98-95-3				
1.80	D	104						
1.83	D	108	23	SF	RC	W	Both	
*1.85	D	30,46	25	SF	AS	W	AQ	
1.85	D	86	20	SF	AS	W	AQ	46
1.85	D	9,10	25	G	HPLC	W	Both	11
1.85	D	78	30	SF	AS	W	Both	37
1.88	D	104						
1.70	I	121		HPLC				
1.79	?	150						
1.82	I	56		HPLC				
1.83	I	74	25	from UNIFAC activity coefficients				
1.84	I	75	25	from UNIFAC activity coefficients				
1.85	(0.05)	Recommended						
$C_7H_7NO_2$		2-Nitrotoluene		CAS # 88-72-2				
*2.30	D	104						
2.30	(0.25)	Recommended						
$C_7H_7NO_2$		3-Nitrotoluene		CAS # 99-08-1				
2.40	D	104						
*2.45	D	46	25	SF	AS	W	AQ	
2.45	(0.10)	Recommended						
$C_7H_7NO_2$		4-Nitrotoluene		CAS # 99-99-0				
*2.37	D	46	25	SF	AS	W	AQ	
2.42	D	104						
2.42	(0.10)	Recommended						
$C_7H_7NO_2$		Phenylnitromethane		CAS # 622-42-4				
*1.75	D	104						
1.75	(0.35)	Recommended						

Table 18. Amides

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
CH_3NO	Methanamide (formamide)			CAS # 75-12-7				
*-1.51	D	104						
-1.51 (0.30) Recommended								
C_2H_5NO	Ethanamide (acetamide)			CAS # 60-35-5				
*-1.26	D	104						
-1.26	D	258		SF	GLC	W	ORG	46
-1.15	D	202	25	SF	RC	pH1		
-1.09	D	156		SF	RC	a	Both	
-1.26 (0.10) Recommended								
C_3H_5NO	Propenamide (acrylamide)			CAS # 79-06-1				
-0.90	D	218		SF				
*-0.67	D	104						
-1.24?	I	144		HPLC				
-0.78 (0.13) Recommended								
C_3H_7NO	N,N-Dimethylmethanamide			CAS # 68-12-2				
*-1.01	D	104						
-1.01 (0.20) Recommended								
C_3H_7NO	N-Methylethanamide			CAS # 79-16-3				
-1.10	D	202	25	SF	RC	pH1		
*-1.05	D	104						
-1.05 (0.10) Recommended								
C_4H_9NO	Butanamide			CAS # 541-35-5				
*-0.21	D	111		SF	CR	W	one	46
-0.21 (0.10) Recommended								
C_4H_9NO	N,N-Dimethylethanamide			CAS # 127-19-5				
-0.77	D	202	25	SF	RC	pH1		
*-0.77	D	104						
-0.77 (0.10) Recommended								

Table 18. Amides (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
$C_6H_{13}NO$	N,N-Diethylethanamide			CAS # 685-91-6				
*0.34	D	104						
0.34	(0.12)	Recommended						
C_7H_7NO	Benzamide			CAS # 55-21-0				
*0.64	D	46	25	SF	AS	W	AQ	
0.64	D	258		SF	GLC	W	AQ	46
0.65	D	104						
0.66	D	154		SF	AS			
0.69	D	260	22	SF	AS	pH9.2	AQ	
0.70	D	260	22	SF	AS	pH3	AQ	
0.84	I	121		HPLC				
0.64	(0.06)	Recommended						
C_7H_7NO	N-Phenylmethanamide	(formanilide)		CAS # 103-70-8				
1.12	D	259	25	SF	AS	W	Both	
*1.15	D	104						
1.26	D	104						
1.00	I	57		HPLC				
1.15	(0.15)	Recommended						
C_8H_9NO	Phenylethanamide			CAS # 103-81-1				
*0.45	D	120		SF	AS	W	AQ	46
0.45	0.10)	Recommended						
C_8H_9NO	3-Methylbenzamide			CAS # 618-47-3				
*1.18	D	104						
1.18	(0.20)	Recommended						
C_8H_9NO	N-(4-Methylphenyl)methanamide			CAS # 3085-54-9				
*1.61	D	259	25	SF	AS	W	Both	
1.61	(0.25)	Recommended						

Table 18. Amides (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_8H_9NO	N-Phenylethanamide (acetanilide)			CAS # 103-84-4				
1.15	D	104				pH3.1		
*1.16	D	46	25	SF	AS	W	AQ	
1.16	D	86	20	SF	AS	W	AQ	46
1.17	D	104						
1.17	D	104						
1.36	D	104						
1.14	I	60		HPLC				
1.16	I	57		HPLC				
1.27[b]	I	64		HPLC				
1.16 (0.05) Recommended								
C_8H_9NO	N-Methylbenzamide			CAS # 613-93-4				
*0.86	D	104						
0.86[c]	?	222						
0.86 (0.10) Recommended								
C_8H_9NO	N-Methyl-N-phenylmethanamide			CAS # 3085-54-9				
*1.09	D	104						
1.09 (0.10) Recommended								
C_9H_8NO	N-(2-Methylphenyl)ethanamide			CAS # 120-66-1				
0.84?	D	20		SF	AS	W	ORG	264
1.51 (0.20) Recommended								
C_9H_8NO	N-(3-Methylphenyl)ethanamide			CAS # 537-92-8				
1.59	D	20		SF	AS	W	ORG	264
1.51 (0.20) Recommended								
C_9H_8NO	N-(4-Methylphenyl)ethanamide			CAS # 103-89-9				
1.59	D	20		SF	AS		ORG	264
1.51 (0.20) Recommended								

Table 18. Amides (continued)

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_9H_9NO		3-Phenylpropenamide (cinnamide)			CAS # 621-79-4			
*1.43	D	104						
1.41	?	199						
1.43 (0.15) Recommended								
$C_{12}H_{17}NO$		N,N-Diethyl-2-methylbenzamide			CAS # 2728-04-3			
2.02	D	261	25	SF	HPLC	W	Both	
2.02 (0.20) Recommended								
$C_{13}H_{11}NO$		N-Phenylbenzamide		CAS # 93-98-1				
*2.62	D	104						
2.70	D	104						
2.62 (0.20) Recommended								

[a] Schistosome saline solution.

[b] Average value.

[c] D. E. Leahy and co-workers, personal communication.

Table 19. Sulphur compounds

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_3H_8S		Propanethiol	CAS # 107-03-9					
*1.81	D	104						
1.81	(0.15)	Recommended						
C_4H_4S		Thiophene	CAS # 110-02-1					
*1.81	D	120		SF	AS	W	AQ	46
1.82	D	104						
1.81	(0.20)	Recommended						
$C_4H_{10}S$		Butanethiol	CAS # 109-79-5					
*2.28	D	104						
2.28	(0.25)	Recommended						
$C_4H_{10}S$		3-Thiapentane (diethylsulphide)		CAS # 352-93-2				
*1.95	D	111		SF	AS	W	AQ	46
1.95	(0.20)	Recommended						
C_6H_6S		Thiophenol	CAS # 108-98-5					
*2.52	D	104						
2.52	(0.25)	Recommended						
C_7H_8S		Thiomethylbenzene		CAS # 100-68-5				
*2.74	D	104						
2.74	(0.25)	Recommended						
C_8H_6S		Benzothiophene		CAS # 95-15-8				
3.09	D	40	25	SF	AS	pH7.4	Both	117
*3.12	D	104						
3.12	(0.10)	Recommended						
$C_{12}H_8S$		Dibenzothiophene		CAS # 132-65-0				
*4.38	?	198						
4.38	(0.40)	Recommended						
$C_{12}H_{10}S$		Diphenylsulphide		CAS # 139-66-2				
3.47	D	104						
*4.45	D	104						
4.45	(0.40)	Recommended						

Table 20. Other

Log P	Code	Ref.	Temp.	Equil. Method	Anal. Method	Aq. Phase	Phases Analyzed	Method Ref.
C_2H_6OS		Dimethylsulphoxide		CAS # 67-68-5				
*-1.35	D	104						
-1.35 (0.20)		Recommended						
$C_2H_6O_2S$		Dimethylsulphone		CAS # 67-71-0				
*-1.41	D	104						
-1.41 (0.20)		Recommended						
$C_5H_{10}O_3$		Diethylcarbonate		CAS # 105-58-8				
*1.21	D	104						
1.21 (0.25)		Recommended						
$C_6H_{14}O_2S$		Dipropylsulphone		CAS # 598-03-8				
0.39	D	262	24	SF	GLC	W	ORG	263
1.15 (0.20)		Recommended						
C_7H_8OS		Methylphenylsulphoxide		CAS # 1193-82-4				
*0.55	D	104						
0.55 (0.10)		Recommended						
$C_7H_8O_2S$		Methylphenylsulphone		CAS # 3112-85-4				
0.47	D	111		SF	AS	W	one	46
*0.50	D	104						
0.50 (0.10)		Recommended						
$C_{12}H_{10}N_2$		Azobenzene		CAS # 103-33-3				
*3.82	D	46	25	SF	AS	W	AQ	
3.82	D	86	20	SF	AS	W	AQ	46
3.82 (0.20)		Recommended						
$C_{12}H_{10}OS$		Diphenylsulphoxide		CAS # 945-51-7				
*2.06	D	104						
2.06 (0.20)		Recommended						
$C_{13}H_{10}O_3$		Diphenylcarbonate		CAS # 102-09-0				
*3.28	D	104						
3.28 (0.30)		Recommended						

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