Modeling of tracer diffusion in liquids when solute-solvent interactions are present

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Abstract

The linear solvation energy relationship (LSER) model is employed to correlate the tracer diffusion coefficients of 550 binary systems at 298.15 K. Among the selected solutes and solvents there exist apolar, polar and hydrogen-bonding substances that can interact with themselves (solvent polymerization) or with the other compound (solute-solvent complexes formation). The results of the proposed formulas are compared with those of other predictive equations.

Keywords: Diffusivity; Interactions; Polymerization; Complexation; LSER

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1. Introducción

In mass transfer operations, equilibrium data and diffusion coefficients are indispensable. In binary liquid mixtures at low pressures, fluid phase equilibria can be roughly predicted by the UNIFAC group contribution method [1], but there is not yet a fully predictive method for binary diffusivities. Equations as those of Li et al. [2] and Bosse and Bart [3] can deal with highly non-ideal systems, but they need good equilibrium data and tracer diffusion coefficients. These tracer diffusivities, so-called binary diffusion coefficients at infinite dilution or limiting binary diffusivities are determined by several factors, and they turn into the solvent self-diffusion coefficients when the solute and solvent molecules become equal.

Easteal and Woolf [4] measured the binary diffusivities at atmospheric pressure of several solutes in acetonitrile, toluene, hexane and water at 298.15 K and in octamethylcyclotetrasiloxane at 323.15 K and represented D_{AB} versus the inverse value of solute diameter, according the Stokes-Einstein equation. In the slightly polar toluene, all data were placed on the same straight line, and in the very polar acetonitrile, the solutes were distributed on two lines: one for apolar or slightly polar solutes and another for highly polar solutes. In water and octamethylcyclotetraxilosane, there were also two lines, but according the ability of hydrogen-bonding formation between solvent and solute. Besides, in octamethylcyclotetraxilosane the lines were not straight, but logarithmic. In hexane, an apolar molecule, there were two lines, but these were not related with the polarity, and Easteal and Woolf were unable to explain this surprising fact.

Care must be taken whit these results of Easteal and Woolf, because the solutes have different masses, sizes and shapes. Chan [5] investigate the diffusion of CCl_4, $(CH_3)CCl_3$, $(CH_3)_2CCl_2$, $(CH_3)_3CCl$ and $(CH_3)_4C$ in acetone, methanol, ethanol and n-decane at atmospheric pressure and

298.15 K, observing that the diffusion coefficients were nearly the same for all solutes in each solvent. The above-mentioned solutes have sizes and shapes very similar, but different masses and dipolar moments, so Chan concluded that these two last variables did not influence the molecular movement (which is in contradiction with Easteal-Woolf and Codastefano et al. [6]). Chan also analysed the shape influence in another work [7]. The chosen solutes were the three xylenes, the three dichlorobenzenes, the p-chlorotoluene and the tetramethyl tin, all being planar molecules of similar size, except the tin derivative, which is spherical. In the three solvents selected, acetone, ethanol and n-tetradecane only the geometry was important: D_{AB} was smaller for $(CH_3)_4Sn$ than for the rest. Among the disubstituted benzenes, the tendency was *ortho*<*meta*<*para* , which is the same of spherical<planar<lineal. This tendency coincides with the research of Hayduck and Buckley in CCl_4 and *n*-hexane [8], and with the work of Tyrrell in propylenglicol and hexylenglicol [9,10]. Nevertheless, the shape effect is less pronounced when the solvent molecules are bigger: Chan and Chan measured the diffusivities of planar and spherical solutes with different sizes in acetone, ethanol and *n*-tetradecane [11] and observed that the planar molecules did not move more quickly than spherical molecules with the same volume in acetone, in contrast with its movement in ethanol and n-tetradecane.

The geometry is also very important in the specific interactions [12]. The diffusivities of 1,3- and 1,4-cyclohexanediol in ethanol are 26% less than 1,2-cyclohexanodiol, and the diffusion of 1,3,5-cyclohexanetriol is 32% less than the 1,2,3-cyclohexanetriol. The movility of the trans-isomer of cyclopentane-1,2-diol is 21% less than the cis isomer, and all is due to the formation of intramolecular hydrogen-bonds because the spatial distribution of hydroxil groups, so the molecules are unable of forming hydrogen bonds with the solvent. The tendency orto<meta<para is inverted when aminopyridines, dihydroxibenzenes, nitrophenols and nitroanilines diffuse in ethanol [13] because of these intramolecular hydrogen bonds. Besides, if the solute molecule has a compact structure, the area per unit volume is less, and the friction with the solvent is less too,

so this effect can counteract the hydrogen bond formation, as occurs with cyclic ethers in water [14]: in a ring of six members is expected that the diffusivity decreases when the -CH_2- groups are substituted by -O-, but the opposite trend is observed.

Easteal [15] systematically studied the diffusion of water in a wide variety of solvents at 298.15 K: ethers, alkylbenzenes, dichlorobenzene, nitrobenzene, formamide and its derivatives, nitriles, alcohols, acetone, dimethyl sulfoxide, cyclohexane, hexane, CCl_4 and *N*-methylpirrolidone. He observed that the product (binary diffusion × solvent viscosity) in benzene derivatives, cyclohexane, hexane and CCl_4 is four times bigger than in the other solvents, and the viscosity dependence of D_{AB} differs from the two groups of solvents.

On the other hand, classic predictive equations as Wilke-Chang [1], Tyn-Calus [16] and Hayduk-Minhas [17] do not take into account solute-solvent interactions, or only consider them in a superficial way. They focuse in the effect of the solvent hydrogen-bonding. The expression of Nakanishi [18] is probably the only one that introduces these effects through empirical corrective parameters, whereas Lusis and Ratcliff [19], Kuppuswamy and Laddha [20] and Mohan and Srnivasan [21] treat solvent polymerization and solute-solvent complexation as chemical reactions, with equilibrium constants that are not easily available.

In this work, the linear solvation energy relationship (LSER) has been applied to tracer diffusivities in liquids at 298.15 K. LSER has many well-known parameters for specific interactions and has been used to model partition coefficients [22], chromatographyc retention volumes [23], limiting activity coefficients [24] and solubilities of solids in supercritical carbon dioxide [25]. The analogy between limiting activity coefficients and tracer diffusivities (an isolated different particle in a homogeneus medium) is a sign that this relationship can correlate binary diffusion coefficients at infinite dilution.

2. Simple equations for predicting tracer diffusion in liquids

All of these are based in the Stokes-Einstein expression. According to this, the diffusion of one spherical particle *A* in a continuum solvent *B* is

$$D_{AB} = \frac{kT}{3\pi\sigma_A\eta_B} \tag{1}$$

where k is the Boltzmann constant (1.380658×10^{-23} J/K), T the absolute temperature, η_B the solvent viscosity and σ_A the molecular diameter of the solute. In principle, Eq.(1) can only be applied when the solute molecules are much larger than the solvent ones.

The Wilke-Chang is the most known of these equations [1]. These authors fitted a lot of experimental diffusivities to the formula

$$D_{AB} = \frac{5.88\times10^{-17}T\sqrt{M_B f_B}}{\eta_B V_{bA}^{0.6}} \tag{2}$$

where M_B is the solvent molecular weight, V_{bA} the molar volume of solute at the normal boiling point and f_B an empirical association factor which takes the values of 2.6 for water, 1.9 for methanol, 1.5 for ethanol and 1.0 for non-associated solvents. When the solute is water, it is assumed to diffuses as a tetramer [26].

On the other hand, Hayduk and Minhas [17] proposed

$$D_{AB} = 4.364\times10^{-18}\frac{T^{1.7}}{\eta_B^{0.8}}\left(\frac{r_{gB}^{0.2}}{r_{gA}^{0.4}}\right) \tag{3}$$

where r_g is the radius of gyration, a measure of the molecular size and sphericity. Instead of this magnitude, Kooijman [27] introduces in Eq. (1) the surface and volume parameters of UNIFAC, *Q* and *R*, respectively, to take into account the shape and the size of the solute and the solvent.

$$D_{AB} = 1.58\left(1-\left|1-\frac{R_A/Q_A}{1.249}\right|\right)\sqrt[3]{1-\left|1-\frac{R_B/Q_B}{1.249}\right|}\left[1+\left(\frac{R_B}{R_A}\right)^{1/3}\right]\frac{kT}{3\pi\eta_B\sigma_A} \tag{4}$$

$$\sigma_A = 6.36\times10^{-10}R_A^{1/3} \tag{5}$$

The constant 1.249 is a reference value, obtaining from the cocient *R*/*Q* for the functional group –CH_2-. No association factor or water teramerization have to be considered. When the solute is bigger than the solvent, the size corrective term, 1+ $(R_B/R_A)^{1/3}$ tends to the unity. Nevertheless, as R_A and Q_A are the same for several isomers, Eq. (4) do not differentiate their diffusivities [7], and when the molecules are spherical, the terms inside the absolute value brackets do not tend to zero. Otherwise, Kooijman refited *Q* for carbon tetrachloride and methane, now being 2.40 and 0.938 respectively.

Tyn and Calus [16] employed the parachors of the two components, Γ_i , as a measure of intermolecular forces

$$D_{AB} = 8.93\times10^{-16}\frac{T}{\eta_B}\left(\frac{V_{bA}^{1/6}}{V_{bB}^{1/3}}\right)\left(\frac{\Gamma_B}{\Gamma_A}\right)^{0.6} \tag{6}$$

The parachor is related with the surface tension, and can be calculated from a group contribution method [1, 28] or from the radius of gyration as [29]:

$$\Gamma = 0.1778\times10^{-6}\left(50 + 7.6\times10^{10}r_g+13.75\times10^{20}r_g^2\right) \quad (7)$$

Eq. (6) can not be applied to highly viscous solvents (η_B > 20×10^{-3} to 30×10^{-3} kg.m^{-1}.s^{-1}) and it has to be taken into account that

- If the solute is water, it diffuses as dimer, so V_{bA} and Γ_A have to be multiplied by two.
- If the solute is a carboxilic acid, it diffuses as dimer, except if the solvent is water, methanol or butanol.
- For diffusion of inert solutes in monohydroxy alcohol, V_{bB} and Γ_B have to be multiplied by $8000\,\eta_B$.

Hayduk and Minhas [17] empirically improved the expression of Tyn and Calus and proposed Eq. (8), which is subjet to the same restrictions of solvent viscosity, diffusion of water, acids and inerts in alcohols:

$$D_{AB} = 3.89\times10^{-16}\,\frac{T^{1.29}}{\eta_B^{0.92}}\left(\frac{1}{V_{bB}^{0.23}}\right)\left(\frac{\Gamma_B^{0.5}}{\Gamma_A^{0.42}}\right) \quad (8)$$

Finally, the equation of Nakanishi [18] adds four empirical parameters for representing the solute-solvent interactions: j_i, s_i, a_i and q_i, the values of which are in Table 1.

$$D_{AB} = \frac{T}{\eta_B}\left[\frac{9.97\times10^{-17}}{(j_A q_A V_{298A})^{1/3}} + \frac{2.4\times10^{-15} a_B s_B V_{298B}}{j_A s_A q_A V_{298A}}\right] \quad (9)$$

V_{298A} y V_{298B} are the molar volumes of solute and solvent at 298.16 K and 0.1 MPa. If the solute is solid at these conditions, it is recommended to calculate it as V_{298A} =0.894V_{bA}, and if the solute is gas, V_{298B} =1.065V_{bA}.

For a given solute–solvent combination, all these equations suggest that the group $D_{AB}\eta_B/T$ is constant at atmospheric pressure, but this is in general not true. Hayduk y Cheng [30] analyzed many experimental data and concluded that $D_{AB} = C_1\eta_B^{C_2}$, where the constants C_1 and C_2 were only solute dependent if there was not complex formation. Nevertheless, sometimes C_1 and C_2 vary from solvent to solvent in absence of strong interactions: this is the case of heptane and decane in alkanes of alkanols [31], of some solutes in methanol, 1-butanol and 1-octanol [32] and of oxygen and policyclic aromatic compounds in alkanes or cycloalkanes [33].

Tominaga et al. observed that benzene derivatives [34, 35] and alcohols [36] verify the constancy of $D_{AB}\eta_B/T$ when the solvent is water along the saturation liquid branch, which is strange, because at low temperatures hydrogen-bond formation and complexation are favoured and the effect of bond rupture would be seen at higher temperatures.

3. Proposed general correlation

The LSER model states that any property of a solute *A* in a solvent *B* at given conditions can be written as a linear combination of several solute parameters as

$$\text{Property} = G_0 + G_1 Log L_A^{16} + G_2 \Delta R_A + G_3 \pi_A^* + G_4 \alpha_A^H + G_5 \beta_A^H \quad (10)$$

where G_i are solvent-dependent functions that vary with temperature and pressure. L^{16} is the gas/hexadecane partition coefficient at 298.15 K, ΔR the excess index of refraction (difference between the index of the substance and the index of the alkane with the same molecular volume), π^* represents the dipolarity and polarizability, α^H is the acidity of hydrogen bonds (donor ability of the substance in the bonds) and β^H the basicity of hydrogen bonds (acceptor ability in the bonds). L^{16} is related with the energy of forming a cavity between the solvent molecules for accommodating the solute molecule, and depends on solute size and the cohesiveness of the solvent [24]; ΔR describes the ability of the solute to interact with the solvent through the electrons π and n [37] and π^* is related with the dipole-dipole or dipole-induced dipole interactions between solute and solvent [38]. Sometimes L^{16} is replaced by a characteristic volume of the substance called volume of McGowan [22, 38] and ΔR by an empirical polarity parameter [37, 39].

π^*, α^H and β^H are called solvatochromic parameters, and take values between 0 and 1 for most of the molecules, being determined by chromatographic or spectroscopic techniques. Nevertheless, they are not absolute values, but defined according to several scales, as those of Kamlet-Taft [39,40] and Abraham and co-workers [22, 38]. The three parameters are pressure and temperature dependent, which is a problem for developing formulas as Eq. (10) aplicable in wide ranges of temperatures and pressures [41-47].

We are not the first that have employed LSER for tracer diffusion. Wang et al. [48] and Chan and coworkers [49,50] developed expressions for these, although with limitations.

The equation of Wang et al. is only valid for carbon dioxide in the ranges 313<*T*<333 K and 8<*P*<30 MPa. The functions G_i are taken constant, but the density and temperature dependent is introducted as Lagalante and Bruno [51], through the dipolarity/polarizability of the solvent:

$$logD_{AB} = \text{-}8.0289 - 0.0011LogL_A^{16} - 0.0209\Delta R_A - 0.1226\pi_A^* - 0.0088\alpha_A^H + 0.1951\beta_A^H - 2.2988\pi_B^* \quad (11)$$

$$\pi_B^* = 1.15\rho_{rB} - 0.98 \quad \text{if} \quad \rho_{rB} < 0.7$$
$$\pi_B^* = 0.173\rho_{rB} - 0.37 \quad \text{if} \quad \rho_{rB} > 0.7 \quad (12)$$

Lu et al. [49] and Chen et al. [50] only used α^H and β^H for studying the interactions of benzene derivatives in ethanol and acetone at 298.15 K. Empirically, they observed that the diffusivities of substances that did not form complexes with the solvents (*nhb*) were related with the diffusivities of complex-forming substances (*assoc*) with the same molecular volume as

$$\left(\frac{1}{D_{AB}}\right)^{assoc} = \left(\frac{1}{D_{AB}}\right)^{nhb} + \left[C_1\alpha_A^H + C_2\beta_A^H\right] \quad (13)$$

where C_1=0.153×10^{-9} m^{-2}. s and C_2=0.0 for acetone and C_1=0.287×10^{-9} m^{-2}. s and C_2=0.079×10^{-9} m^{-2}.s for ethanol. The solutes included nitrophenols, dihydroxibenzenes, methylanilines, substituded benzoic acids, etc.

A supplementary Table compiles the data for the present work: 914 points of 510 binary systems at 298.15 K, including solvent self-diffusivities. Some points in octane and in

chloroform that were at temperatures close to it were taken too. When experimental diffusivities of several authors for the same system were very different, these were disregarded. Table 2 shows the properties of solutes and solvents necessary for calculations, most of them taken from the Korea Thermophysical Property Data Bank (KDB), which website is http://www.cheric.org/kdb/ , and from the database of the software HYSYS.

After a lot of trials with the help of the software MICROSOFT FORTRAN POWER STATION 4.0 it was found that fewer errors were obtained with

$$\left[\frac{10^{-12}}{\eta_B D_{AB}}\right]^n = C_{11} + C_{12}\Delta R_B + C_{13}\pi_B^* + C_{14}\alpha_B^H + C_{15}\beta_B^H + C_{16} LogL_B^{16}$$
$$+ \left(C_{21} + C_{22}\Delta R_B + C_{23}\pi_B^* + C_{24}\alpha_B^H + C_{25}\beta_B^H + C_{26} LogL_B^{16}\right)\Delta R_A$$
$$+ \left(C_{31} + C_{32}\Delta R_B + C_{33}\pi_B^* + C_{34}\alpha_B^H + C_{35}\beta_B^H + C_{36} LogL_B^{16}\right)\pi_A^*$$
$$+ \left(C_{41} + C_{42}\Delta R_B + C_{43}\pi_B^* + C_{44}\alpha_B^H + C_{45}\beta_B^H + C_{46} LogL_B^{16}\right)\alpha_A^H$$
$$+ \left(C_{51} + C_{52}\Delta R_B + C_{53}\pi_B^* + C_{54}\alpha_B^H + C_{55}\beta_B^H + C_{56} LogL_B^{16}\right)\Delta\beta_A^H$$
$$+ \left(C_{61} + C_{62}\Delta R_B + C_{63}\pi_B^* + C_{64}\alpha_B^H + C_{65}\beta_B^H + C_{66} LogL_B^{16}\right) LogL_A^{16} \qquad (14)$$

If n = 1, Eq. (14) has the same form as Eq. (13), and the proposed model becomes a Taylor series of the molecular diameter. Nevertheless, it is probable that the diffusivities of some systems not considered in the correlation will be negative, thus n is fixed as 1/2, and the model becomes the Taylor series of σ^2_A (the same exponent as in the Wilke–Chang equation). The parity plots of the two cases are nearly equal, and are shown in Figs. 1 and 2. The values for the C_{ij} obtained from the fits to Eq. (14) are given in Table 3. Eq (14) is similar to that developed by Meyer and Maurer [52], who proposed an empirical formula of 36 fitting constant for the logarithm of the water / any organic solvent partition coefficient. It was not possible to supress

the solvent viscosity, because the average absolute deviation (AAD) rises to 25%, nor to develope an exponential equation instead lineal one, because AAD is 15% (which is near the values of Tyn-Calus and Nakanishi, as can be seen in Table 4).

Eq.(14) with n=1 has the lower AAD, closely followed by its modification with n=1/2. In the first one there are 14 solvents with AAD<10%, and in the second one there are 10 solvents. None of the other formulas studied give such good predictions for so many solvents.

The two versions of Eq. (14) are the best for predicting limiting diffusivities in all alcohols except for isobutanol, because the LSER model incorporates the solute-solvent interactions that Wilke-Chang, Kooijman, Tyn-Calus and Hayduk-Minhas do not take into account and are roughly considered by Nakanishi.

In acetone, the equation of Tyn and Calus is better than the ours. The worst results are obtained for methylcyclohexane, diethyl ether, diethyl ketone, carbon disulfide and isobutanol, in which AAD>30%. Nevertheless, in the other two good equations, Tyn-Calus and Nakanishi, the number of solvents in which this error is surpassed is of 7 and 10 respectively. Besides, the high deviations of Eq. (14) are in solvents in which the number of experimental points are between one and four.

4. Conclusions

Two new predictive equations, based in the linear solvation energy relationship and in the Stokes-Einstein equation have been developed for predicting binary diffusivities at infinite dilution of the solvent at 298.15 K. The solute and solvent descriptors provided by the LSER

model describe the interactions of both substances in the mixture, firstly due to the formation of hydrogen bonds. The average absolute deviations are less than those of formulas like Tyn-Calus or Nakanishi.

List of symbols

a	interaction parameter in the equation of Nakanishi
AAD	average absolute deviation
C	fitting constans
D_{AB}	binary diffusivity at infinite dilution (m^2s^{-1})
f	correction factor in the equation of Wilke-Chang
G_i	mathematical funtions
j	interaction parameter in the equation of Nakanishi
k	Boltzmann constant =1.380658×10^{-23} J K^{-1}molecule^{-1}
$logL^{16}$	logarithm of the gas/hexadecane partition coefficient
M	molar mass, (kg mol^{-1})
q	quantic parameter in the equation of Nakanishi
Q	van der Waals surface parameter
r_g	radius of gyration, m
R	van der Waals volume parameter
ΔR	excess index of refraction
s	interaction parameter in the equation of Nakanishi

T	absolute temperature (K)
V	molar volume (m^3mol^{-1})
V_{298}	molar volume at 298.15 K (m^3mol^{-1})

Greek letters

α^H	donor ability of one substance in hygrogen bonds
β^H	acceptor ability of one substance in hygrogen bonds
Γ	parachor ($kg^{0.25}\ m^3\ mol^{-1}\ s^{-0.5}$)
ΔR	excess index of refraction
η	viscosity ($kg\ m^{-1}s^{-1}$)
μ_p	dipolar moment (Debye)
π^*	dipolarity/polarizability parameter
ρ	density ($kg\ m^{-3}$)
σ	molecular diameter (m)

Superscripts

assoc	referred to complex-forming substances
nhb	referred to substances that do not form complexes

Subscripts

A	solute
B	solvent
b	normal boiling point
m	melting point
r	reduced property

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Appendix A. Supplementary data

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FIGURES

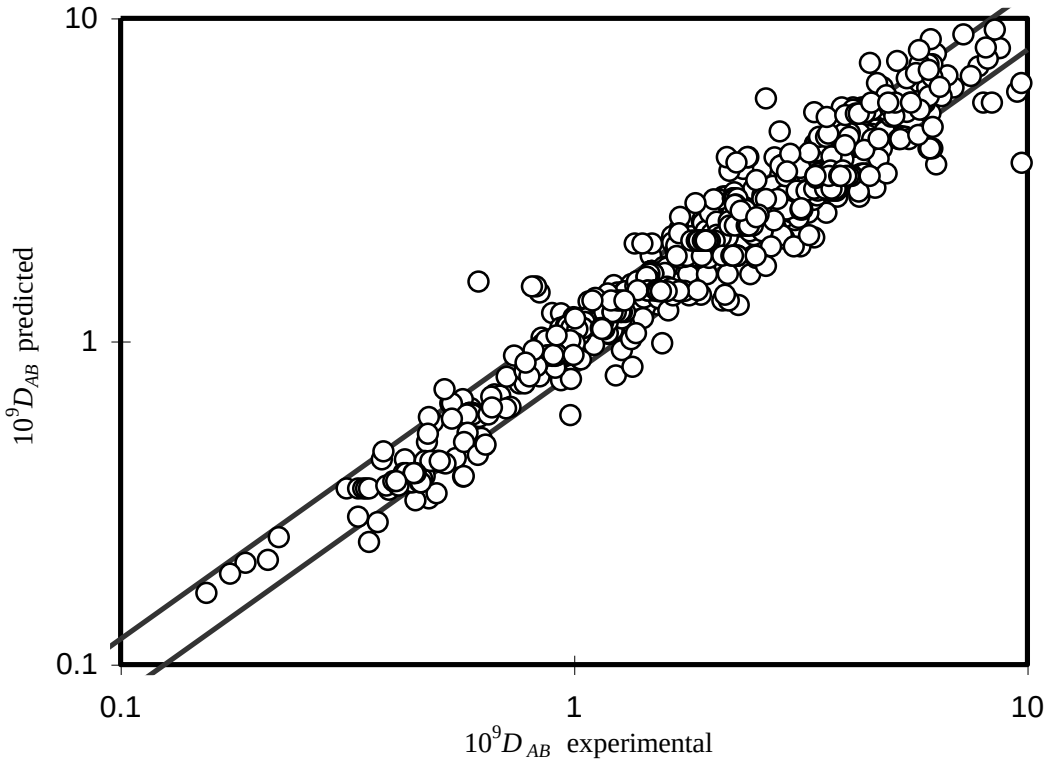

Fig.1. Parity plot for Eq. (14) with *n*=1.

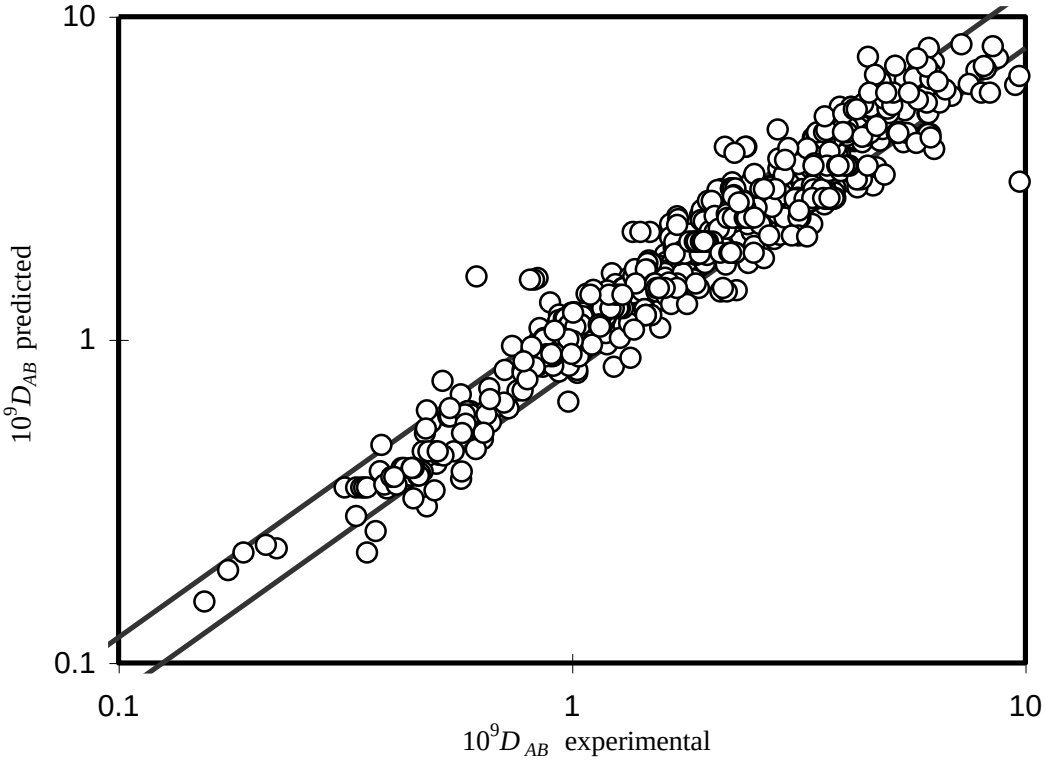

Fig.2. Parity plot for Eq. (14) with n=1/2.

TABLES

Table 1
Parameters of Nakanishi

Substance(s)	As solutes (*A*)			As solvents (*B*)	
	j_A	s_A	q_A	a_B	s_B
Water	2.8 (1.8) [a]	1.0	1.0	2.8	1.0
methanol	2.2 (1.5)	1.0	1.0	2.0	1.0
ethanol	2.5 (1.5)	1.0	1.0	2.0	1.0
Other aliphatic monohydric alcohols	1.5	1.0	1.0	1.8	1.0
Glycols, organic acids and other associated compounds	2.0	1.0	1.0	2.0	1.0
Hygly polar substances (iodine, pyridine, aniline, nitrobenzene...)	1.5	1.0	1.0	1.0	1.0
Paraffins (C_5-C_{12})	1.0	0.7	1.0	1.0	0.7
Quantum gases			$1+0.85(\Lambda_A^*)^2$ [b]		
Other substances	1.0	1.0	1.0	1.0	1.0

[a] The values in parentheses are for cases where the solvents are more polar than the solute.
[b] Λ^* is 3.08 for He^3, 2.67 for He^4, 1.729 for H_2, 1.223 for D_2, 0.593 for Ne and zero for all other substances.

Table 2

Properties of solutes and solvents studied in this work

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K) [a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K) [a, c]	r_g (Å) [a, d]	μ_p (Debyes) [a]	R [e]	Q [e]	ΔR [f]	π^* [f]	α^H [f]	β^H [f]	$log\ L^{16}$ [f]
Methane	CH_4	16.04	111.67	37.97	40.44	90.66	1.123	0.00	1.1292	1.124	0.000	0.00	0.00	0.00	-0.323
Ethane	C_2H_6	30.07	184.50	55.22	58.81	89.88	1.831	0.00	1.8022	1.696	0.000	0.00	0.00	0.00	0.492
Propane	C_3H_8	44.10	231.00	75.68	80.60	85.44	2.426	0.00	2.4766	2.236	0.000	0.00	0.00	0.00	1.050
n-Butane	C_4H_{10}	58.12	272.60	96.47	102.75	134.86	2.889	0.00	3.1510	2.776	0.000	0.00	0.00	0.00	1.615
n-Pentane	C_5H_{12}	72.15	309.21	118.19	116.05	143.40	3.385	0.00	3.8254	3.316	0.000	0.00	0.00	0.00	2.162
n-Hexane	C_6H_{14}	86.18	341.88	140.21	131.36	177.84	3.812	0.00	4.4998	3.856	0.000	0.00	0.00	0.00	2.668
n-Heptane	C_7H_{16}	100.20	371.60	163.03	147.03	182.57	4.267	0.00	5.1742	4.396	0.000	0.00	0.00	0.00	3.173
n-Octane	C_8H_{18}	114.23	398.82	186.68	163.38	216.38	4.680	0.00	5.8486	4.936	0.000	0.00	0.00	0.00	3.677
n-Nonane	C_9H_{20}	128.26	423.97	210.58	179.56	219.66	4.985	0.00	6.5230	5.476	0.000	0.00	0.00	0.00	4.182
n-Decane	$C_{10}H_{22}$	142.28	447.30	235.96	195.83	185.34	5.539	0.00	7.1974	6.016	0.000	0.00	0.00	0.00	4.686
n-Dodecane	$C_{12}H_{26}$	170.34	489.47	287.29	228.61	211.28	5.914	0.00	8.5462	7.096	0.000	0.00	0.00	0.00	5.696
n-Tetradecane	$C_{14}H_{30}$	198.39	526.73	341.67	261.27	255.01	6.621	0.00	9.8950	8.176	0.000	0.00	0.00	0.00	6.705
n-Hexadecane	$C_{16}H_{34}$	226.45	560.01	397.37	294.22	291.34	7.063	0.00	11.2438	9.256	0.000	0.00	0.00	0.00	7.714
n-Octadecane	$C_{18}H_{38}$	254.50	589.50	453.73	327.39	301.30	7.655	0.00	12.5926	10.336	0.000	0.00	0.00	0.00	8.722
n-Eicosane	$C_{20}H_{42}$	282.54	616.93	476.45	425.95	309.90	8.364		13.9414	11.416	0.000	0.00	0.00	0.00	9.731
n-Docosane	$C_{22}H_{46}$	310.59	641.76	523.18	467.72	317.16	7.559		15.2902	12.496	0.000	0.00	0.00	0.00	10.740
Neopentane (2,2-dimetylpropane)	C_5H_{12}	72.15	282.63	119.73	127.51	256.50	3.318	0.00	3.8239	3.392	0.000	0.00	0.00	0.00	1.820
Isopentane (2-methylbutane)	C_5H_{12}	72.15	301.03	117.67	117.10	113.20	3.313	0.10	3.8246	3.312	0.000	0.00	0.00	0.00	2.013

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K)[a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K)[a, c]	r_g (Å)[a, d]	μ_p (Debyes)[a]	R[e]	Q[e]	ΔR[f]	π^*[f]	α^H[f]	β^H[f]	$log\ L^{16}$[f]
2,2-Dimethylbutane	C_6H_{14}	86.18	322.88	138.84	133.78	174.00	3.476		4.4983	3.932	0.000	0.00	0.00	0.00	2.352
2,2,4-Trimethylpentane (isooctane)	C_8H_{18}	114.23	372.37	182.94	165.45	165.80	4.171		5.8463	5.008	0.000	0.00	0.00	0.00	3.106
Ethylene	C_2H_4	28.05	169.38	49.32	52.52	104.00	1.538	0.00	1.5700	1.490	0.107	0.10	0.00	0.07	0.289
Propylene	C_3H_6	42.08	225.46	68.96	73.44	87.90	2.228	0.40	2.2465	2.024	0.103	0.08	0.00	0.07	0.946
Cyclopentane	C_5H_{10}	70.13	322.40	97.46	94.61	179.30	3.120	0.00	3.3720	2.700	0.263	0.10	0.00	0.00	2.477
Methylcyclopentane	C_6H_{12}	84.16	344.90	120.41	113.04	130.60	3.167	0.00	4.0456	3.236	0.225	0.10	0.00	0.00	2.816
Cyclohexane	C_6H_{12}	84.16	353.88	116.80	108.86	279.83	3.261	0.30	4.0464	3.240	0.305	0.10	0.00	0.00	2.964
Methylcyclohexane	C_7H_{14}	98.19	374.08	141.04	128.19	146.50	3.747	0.00	4.7200	3.776	0.244	0.10	0.00	0.00	3.323
Cyclooctane	C_8H_{16}	112.21	422.00	153.61	134.87	287.98	4.098		5.3952	4.320	0.413	0.10	0.00	0.00	4.329
Benzene	C_6H_6	78.11	353.24	95.82	89.48	278.69	3.004	0.00	3.1878	2.400	0.610	0.52	0.00	0.14	2.786
Toluene	C_7H_8	92.14	383.78	118.02	106.57	178.18	3.443	0.40	3.9228	2.968	0.601	0.52	0.00	0.14	3.325
o-Xylene	C_8H_{10}	106.17	417.60	137.91	121.15	247.98	3.789	0.50	4.6578	3.536	0.663	0.56	0.00	0.16	3.939
m-Xylene	C_8H_{10}	106.17	412.27	140.30	123.39	225.30	3.897	0.30	4.6578	3.536	0.623	0.52	0.00	0.16	3.839
p-Xylene	C_8H_{10}	106.17	411.52	140.98	123.92	286.41	3.796	0.10	4.6578	3.536	0.613	0.52	0.00	0.16	3.839
1,2,4-Trimethylbenzene	C_9H_{12}	120.19	442.53	160.96	137.80	229.30	4.199		5.3928	4.104	0.677	0.56	0.00	0.19	4.441
1,3,5-Trimethylbenzene (mesitylene)	C_9H_{12}	120.19	437.89	163.13	139.54	228.40	4.341	0.10	5.3928	4.104	0.649	0.52	0.00	0.19	4.344
Ethylbenzene	C_8H_{10}	106.17	409.34	139.52	122.76	178.20	3.821	0.40	4.5972	3.508	0.613	0.51	0.00	0.15	3.778
Propylbenzene	C_9H_{12}	120.19	432.39	162.72	139.79	173.59	4.194		5.2716	4.048	0.604	0.50	0.00	0.15	4.230
Isopropylbenzene (cumene)	C_9H_{12}	120.19	425.56	162.00	139.86	177.14	4.322		5.2708	4.044	0.602	0.49	0.00	0.16	4.084
Butylbenzene	$C_{10}H_{14}$	134.22	456.46	190.82	156.07	185.20	4.849	0.40	5.9460	4.588	0.600	0.51	0.00	0.15	4.730
Isobutylbenzene	$C_{10}H_{14}$	134.22	445.94	183.99	157.35	221.70	4.555	0.30	5.9452	4.584	0.580	0.47	0.00	0.15	4.500
tert-Butylbenzene	$C_{10}H_{14}$	134.22	442.30	176.27	155.53	215.30	4.318	0.50	5.9445	4.664	0.619	0.49	0.00	0.16	4.413

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K)[a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K)[a, c]	r_g (Å)[a, d]	μ_p (Debyes)[a]	R[e]	Q[e]	ΔR[f]	π^*[f]	α^H[f]	β^H[f]	$log\ L^{16}$[f]
sec-Butylbenzene (2-phenylbutane)	$C_{10}H_{14}$	134.22	446.54	183.33	154.81	197.70	4.564	0.40	5.9452	4.584	0.603	0.48	0.00	0.16	4.506
Naphthalene	$C_{10}H_8$	128.17	491.14	154.77	138.37	353.30	4.045	0.00	4.9808	3.440	1.340	0.92	0.00	0.20	5.161
1-Methylnaphthalene	$C_{11}H_{10}$	142.20	517.83	201.30	179.96	242.67	4.435	0.50	5.7158	4.008	1.344	0.90	0.00	0.20	5.789
1-Ethylnaphthalene	$C_{12}H_{12}$	156.23	531.50	200.69	179.42	259.00	4.657		6.3902	4.548	1.371	0.87	0.00	0.20	6.136
Biphenyl	$C_{12}H_{10}$	152.21	529.20	190.82	170.59	342.00	4.834		6.0434	4.240	1.360	0.99	0.00	0.22	6.014
Biphenylmethane	$C_{13}H_{12}$	168.24	538.20	217.46	194.41	298.39	4.935	0.40	6.7178	4.780	1.220	1.04	0.00	0.28	6.313
Phenanthrene	$C_{14}H_{10}$	178.23	613.45	213.82	191.15	372.39	4.980	0.00	6.7738	4.480	2.055	1.29	0.00	0.26	7.632
Anthracene	$C_{14}H_{10}$	178.23	615.18	213.82	191.15	489.70	4.980	0.00	6.7738	4.480	2.290	1.34	0.00	0.26	7.568
Pyrene	$C_{16}H_{10}$	202.26	666.00	243.03	217.27	423.80	5.152		7.5042	4.720	2.808	1.71	0.00	0.29	8.833
Diethyl ether	$(C_2H_5)_2O$	74.12	307.60	106.37	104.69	156.80	3.140	1.30	3.3949	3.016	0.041	0.25	0.00	0.45	2.015
Anisol (methyl phenyl ether)	C_7H_8O	108.14	426.80	125.32	109.17	235.65	3.690	1.20	4.1667	3.208	0.708	0.74	0.00	0.29	3.089
Tetrahydrofurane	C_4H_8O	72.11	338.00	85.91	81.72	165.16	2.600	1.70	2.9415	2.400	0.289	0.52	0.00	0.48	2.636
1,4-Dioxane	$C_4H_8O_2$	88.11	374.60	89.94	85.81	285.00	3.110	0.40	3.1854	2.640	0.329	0.75	0.00	0.64	2.892
Acetone	C_2H_6O	58.08	329.20	77.44	73.84	178.20	2.740	2.90	2.5735	2.336	0.179	0.70	0.04	0.51	1.696
2-Butanone (methyl ethy ketone)	C_4H_8O	72.11	352.74	97.88	90.19	186.48	3.135	3.30	3.2479	2.876	0.166	0.70	0.00	0.51	2.287
Methyl isobutyl ketone	$C_6H_{12}O$	100.16	389.60	141.57	125.80	189.00	3.828	2.80	4.5959	3.952	0.111	0.65	0.00	0.51	3.089
Acetophenone (methyl phenyl ketone)	C_8H_8O	120.15	475.00	140.10	117.37	293.00	3.938	3.00	4.6941	3.608	0.818	1.01	0.00	0.49	4.501
Cyclohexanone	$C_6H_{10}O$	98.14	428.58	119.76	104.17	242.00	3.410	3.10	4.1433	3.340	0.403	0.86	0.00	0.56	3.792
Benzaldehyde	C_7H_6O	106.12	451.90	121.87	101.65	247.00	3.751	2.80	4.0197	3.068	0.820	1.00	0.00	0.39	4.008
Ethyl acetate	$C_4H_8O_2$	88.11	350.26	106.33	98.60	189.50	3.348	1.90	3.4786	3.116	0.106	0.62	0.00	0.45	2.314
Butyl acetate	$C_6H_{12}O_2$	116.16	399.20	152.29	132.59	195.00	4.170	1.80	4.8274	4.196	0.071	0.60	0.00	0.45	3.353
Pyridine	C_5H_5N	79.10	388.38	89.86	80.88	231.50	3.050	2.30	2.9993	2.113	0.631	0.84	0.00	0.52	3.022

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K)[a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K)[a, c]	r_g (Å)[a, d]	μ_p (Debyes)[a]	R[e]	Q[e]	ΔR[f]	π^*[f]	α^H[f]	β^H[f]	$\log L^{16}$[f]
Pyrazine	$C_4H_4N_2$	80.09	389.15	102.24	91.40	326.00	2.873	0.24	2.8108	1.826	0.629	0.95	0.00	0.62	2.920
Acetonitrile	C_2H_3N	41.05	354.80	57.56	52.86	229.32	1.821	3.50	1.8701	1.724	0.237	0.90	0.04	0.33	1.739
Benzonitrile	C_7H_5N	103.12	464.30	132.93	102.10	260.40	3.800	3.50	3.9907	2.996	0.742	1.11	0.00	0.33	4.039
Nitrobenzene	$C_6H_5NO_2$	123.00	481.46	120.93	102.63	278.81	3.944		4.0764	3.104	0.871	1.11	0.00	0.28	4.557
o-Nitrotoluene	$C_7H_7NO_2$	137.14	495.64	168.35	117.92	269.98	4.310	3.75	4.8114	3.672	0.866	1.11	0.00	0.28	4.878
m-Nitrotoluene	$C_7H_7NO_2$	137.14	505.00	168.35	118.53	289.20	4.468	4.23	4.8114	3.672	0.874	1.10	0.00	0.28	5.097
N, N-Dimethylformamide	C_3H_7NO	73.10	426.15	89.53	77.39	212.72	3.027		3.0856	2.736	0.367	1.31	0.00	0.73	3.173
N, N-Dimethylacetamide	C_4H_9NO	87.12	439.25	120.69	92.98	253.16	3.321		3.7601	3.276	0.363	1.33	0.00	0.78	3.717
Carbon tetrafluoride	CF_4	88.00	145.13	53.87	57.37	86.35	2.668	0.00	1.7277	1.760	-0.280	-0.20	0.00	0.00	-0.800
Chloroform	$CHCl_3$	119.38	334.32	84.45	80.51	209.60	3.178	1.10	2.8700	2.410	0.425	0.49	0.15	0.02	2.480
Carbon tetrachloride	CCl_4	153.82	349.90	103.62	97.14	250.00	3.458	0.00	3.3900	2.910	0.458	0.38	0.00	0.00	2.823
Bromoform	$CHBr_3$	252.73	422.45	99.63	87.82	281.20	3.730		3.2945	2.724	0.974	0.68	0.15	0.09	3.784
1,2-Dichloroethane	$C_2H_4Cl_2$	98.96	356.60	85.37	79.45	237.60	2.851	1.80	2.9308	2.528	0.416	0.64	0.10	0.11	2.573
1,1,1-Trichloroethane	$C_2H_3Cl_3$	133.40	347.20	107.99	101.25	238.16	3.373	1.70	3.5412	3.032	0.369	0.41	0.00	0.09	2.733
tert-Butylchloride	C_4H_9Cl	92.57	324.00	114.93	110.71	247.80	3.152	2.10	3.7093	3.268	0.142	0.25	0.00	0.12	2.217
Chlorobenzene	C_6H_5Cl	112.56	404.87	114.46	102.29	227.60	3.568	1.60	3.8127	2.844	0.718	0.65	0.00	0.07	3.657
o-Dichlorobenzene	$C_6H_4Cl_2$	147.00	453.60	136.10	112.56	256.10	4.186	2.30	4.4376	3.288	0.872	0.78	0.00	0.04	4.518
m-Dichlorobenzene	$C_6H_4Cl_2$	147.00	446.23	132.53	114.13	248.39	4.389	1.72	4.4376	3.288	0.847	0.73	0.00	0.02	4.410
p-Dichlorobenzene	$C_6H_4Cl_2$	147.00	447.21	132.53	118.49	326.35	4.149		4.4376	3.288	0.825	0.75	0.00	0.02	4.435
Bromobenzene	C_6H_5Br	157.01	429.21	120.13	105.57	242.30	3.610	1.50	3.9709	2.952	0.882	0.73	0.00	0.09	4.041
Argon	Ar	39.95	87.30	28.66	30.52	83.79	1.076	0.00	1.1050	1.070	0.000	0.00	0.00	0.00	-0.688
Krypton	Kr	83.80	119.93	34.72	36.98	115.94	1.138	0.00	1.3708	1.235	0.000	0.00	0.00	0.00	-0.211

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K) [a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K) [a, c]	r_g (Å) [a, d]	μ_p (Debyes) [a]	R [e]	Q [e]	ΔR [f]	π^* [f]	α^H [f]	β^H [f]	$log\ L^{16}$ [f]
Xenon	Xe	131.29	165.11	44.65	47.55	161.36	1.296	0.00	1.6770	1.415	0.000	0.00	0.00	0.00	0.378
Nitrogen	N_2	28.01	77.36	34.68	36.93	63.14	0.547	0.00	0.9410	0.991	0.000	0.00	0.00	0.00	-0.978
Oxygen	O_2	32.00	90.20	28.02	29.85	54.35	0.604	0.00	0.9130	0.977	0.000	0.00	0.00	0.00	-0.723
Nitrous oxide	N_2O	44.01	184.67	36.00	38.34	182.30	0.954	0.20	1.2407	1.218	0.068	0.35	0.00	0.10	0.164
Carbon monoxide	CO	28.01	81.60	35.42	37.73	68.15	0.558	0.10	1.0600	1.069	0.000	0.00	0.00	0.00	-0.836
Carbon dioxide	CO_2	44.01	194.70	35.02	37.30	216.55	0.992	0.00	1.3000	1.120	0.150	0.42	0.00	0.10	0.057
Sulfur hexafluoride	SF_6	146.05	209.60	73.04	77.79	222.50	2.472		2.9743	2.600	-0.600	-0.20	0.00	0.00	-0.120
Carbon disulfide	CS_2	76.13	319.00	62.26	60.64	161.30	1.424	0.00	2.0570	1.650	0.877	0.21	0.00	0.07	2.353
Hydrogen	H_2	2.02	20.28	28.51	30.37	13.95	0.371	0.00	0.4160	0.570	0.000	0.00	0.00	0.00	-1.200
Water	H_2O	18.02	373.15	18.79	18.06	273.16	0.615	1.80	0.9200	1.400	0.000	0.45	0.82	0.35	0.260
Methanol	CH_3OH	32.04	337.70	42.74	40.58	175.50	1.536	1.70	1.4311	1.432	0.278	0.44	0.43	0.47	0.970
Ethanol	C_2H_5OH	46.07	351.44	62.69	58.62	159.10	2.250	1.70	2.5755	2.588	0.246	0.42	0.37	0.48	1.485
1-Propanol	C_3H_7OH	60.10	370.30	82.07	75.09	146.90	2.736	1.70	3.2499	3.128	0.236	0.42	0.37	0.48	2.031
2-Propanol (isopropanol)	C_3H_7OH	60.10	355.40	82.97	76.90	184.70	2.726	1.70	3.2491	3.124	0.212	0.36	0.33	0.56	1.764
1-Butanol	C_4H_9OH	74.12	390.88	102.67	91.99	183.90	3.225	1.80	3.9243	3.668	0.224	0.42	0.37	0.48	2.601
2-Butanol (*sec*-butanol)	C_4H_9OH	74.12	372.66	100.17	91.99	158.40	3.182	1.70	3.9235	3.664	0.217	0.36	0.33	0.56	2.338
2-Methyl-1-propanol (isobutanol)	C_4H_9OH	74.12	381.04	102.46	92.92	165.00	3.140	1.70	3.9235	3.664	0.217	0.39	0.37	0.48	2.413
2-Methyl-2-propanol (*tert*-butanol)	C_4H_9OH	74.12	355.50	103.67	94.63	298.50	3.019	1.70	3.9228	3.744	0.180	0.30	0.31	0.60	1.963
1-pentanol	$C_5H_{11}OH$	88.15	411.13	123.55	108.53	195.56	3.679	1.70	4.5987	4.208	0.219	0.42	0.37	0.48	3.106
2-Pentanol	$C_5H_{11}OH$	88.15	392.16	121.44	108.56	200.00	3.619		4.5979	4.204	0.195	0.36	0.33	0.56	2.840
3-Pentanol	$C_5H_{11}OH$	88.15	388.46	119.07	106.95	204.00	3.503	1.80	4.5979	4.204	0.218	0.36	0.33	0.56	2.860
2-Methyl-1-butanol	$C_5H_{11}OH$	88.15	401.90	122.00	108.27	203.00	3.612		4.5979	4.204	0.219	0.39	0.37	0.48	3.011

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K)[a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K)[a, c]	r_g (Å)[a, d]	μ_p (Debyes)[a]	R[e]	Q[e]	ΔR[f]	π^*[f]	α^H[f]	β^H[f]	$\log L^{16}$[f]
2-Methyl-2-butanol	$C_5H_{11}OH$	88.15	375.50	124.24	109.50	264.30	3.359	1.90	4.5972	4.284	0.194	0.30	0.31	0.60	2.630
3-Methyl-1-butanol (isoamyl alcohol)	$C_5H_{11}OH$	88.15	405.20	122.60	109.25	155.90	3.684	1.80	4.5979	4.204	0.192	0.39	0.37	0.48	3.011
1-Hexanol	$C_6H_{13}OH$	102.18	430.70	144.33	125.24	228.50	4.144	1.80	5.2731	4.748	0.210	0.42	0.37	0.48	3.610
1-Heptanol	$C_7H_{15}OH$	116.20	449.60	168.18	141.80	239.00	4.380	1.70	5.9475	5.288	0.211	0.42	0.37	0.48	4.115
1-Octanol	$C_8H_{17}OH$	130.23	468.31	191.67	158.48	257.60	4.787	2.00	6.6219	5.828	0.199	0.42	0.37	0.48	4.619
1-Decanol	$C_{10}H_{21}OH$	158.29	506.10	237.72	191.53	280.00	5.500	1.80	7.9707	6.908	0.191	0.42	0.37	0.48	5.628
Cyclopentanol	$C_5H_{10}O$	86.13	413.95	116.55	90.76	254.00	3.375		4.1445	3.588	0.427	0.54	0.32	0.56	3.241
Cyclohexanol	$C_6H_{12}O$	100.16	434.40	122.25	105.75	298.61	3.601	1.70	4.8189	4.128	0.460	0.54	0.32	0.57	3.758
Phenol	C_6H_6O	94.11	434.85	99.42	88.88	314.00	3.550	1.60	3.5517	2.680	0.805	0.89	0.60	0.31	3.766
p-Chlorophenol	C_6H_5ClO	128.56	493.11	122.26	109.30	317.16	3.913	2.11	4.1766	3.124	0.915	1.08	0.67	0.21	4.775
o-Cresol (*o*-methylphenol)	C_7H_8O	108.14	464.19	120.93	103.95	302.90	3.787	1.60	4.2867	3.248	0.840	0.86	0.52	0.31	4.218
p-Cresol	C_7H_8O	108.14	475.13	122.48	105.08	308.90	3.762	1.60	4.2867	3.248	0.820	0.87	0.57	0.32	4.312
2,5-Dimethylphenol (xylenol)	$C_8H_{10}O$	122.17	484.30	179.97	160.89	347.90	4.128	1.50	5.0217	3.816	0.840	0.79	0.54	0.37	4.774
2,6-Dimethylphenol (xylenol)	$C_8H_{10}O$	122.17	474.20	200.09	178.88	318.80	4.068		5.0217	3.816	0.860	0.79	0.39	0.39	4.680
Benzyl alcohol	C_7H_8O	108.14	478.60	112.43	103.48	257.90	3.813	1.70	4.6961	3.860	0.803	0.87	0.33	0.56	4.221
Ammonia	NH_3	17.03	239.82	24.98	26.61	195.41	0.853	1.50	1.0000	1.000	0.139	0.35	0.14	0.62	0.680
Aniline (benzenoamine)	C_6H_7N	93.13	457.32	106.30	91.63	267.13	3.393	1.60	3.7165	2.816	0.955	0.96	0.26	0.50	3.934
o-Nitroaniline	$C_6H_6N_2O_2$	138.13	558.00	154.38	138.01	347.66	4.198	4.06	4.6051	3.520	1.180	1.37	0.30	0.36	5.627
m-Nitroaniline	$C_6H_6N_2O_2$	138.13	579.00	154.38	138.01	386.16	4.350	4.90	4.6051	3.520	1.200	1.71	0.40	0.35	5.880
p-Nitroaniline	$C_6H_6N_2O_2$	138.13	609.15	154.38	138.01	420.15	4.263	6.29	4.6051	3.520	1.220	1.91	0.42	0.38	6.343
p-Chloroaniline	C_6H_6ClN	127.57	503.65	137.68	123.09	343.66	3.929	2.99	4.3414	3.260	1.060	1.13	0.30	0.32	4.889
p-Toluidine (*p*-methylaniline)	C_7H_9N	107.15	473.70	132.14	118.13	316.90	3.783	1.60	4.4515	3.384	0.923	0.95	0.23	0.45	4.452

Substance	Formula	$10^3 M$ (kg/mol)[a]	T_b (K)[a]	$10^6 V_b$ (m^3/mol)[b]	$10^6 V_{298}$ (m^3/mol)[b]	T_m (K)[a, c]	r_g (Å)[a, d]	μ_p (Debyes)[a]	R[e]	Q[e]	ΔR[f]	π^*[f]	α^H[f]	β^H[f]	$log\ L^{16}$[f]
m-Toluidine	C_7H_9N	107.15	476.60	132.14	107.26	241.90	3.876	1.50	4.4515	3.384	0.946	0.95	0.23	0.45	4.463
Acetic acid	$C_2H_4O_2$	60.05	391.00	61.10	57.65	289.80	2.595	1.30	2.2024	2.072	0.265	0.65	0.61	0.45	1.750
Propionic acid	$C_3H_6O_2$	74.08	414.30	81.49	74.97	252.40	3.050	1.50	2.8768	2.612	0.233	0.65	0.60	0.45	2.290
Butyric acid	$C_4H_8O_2$	88.11	436.90	99.73	92.59	267.40	3.610	1.50	3.5512	3.152	0.210	0.62	0.60	0.45	2.830
Valeric (or pentanoic) acid	$C_5H_{10}O_2$	102.13	459.50	128.18	108.76	239.00	3.965		4.2256	3.692	0.205	0.60	0.60	0.45	3.380
Caproic (or hexanoic) acid	$C_6H_{12}O_2$	116.16	478.85	147.61	125.31	270.00	4.404	1.19	4.9000	4.232	0.174	0.60	0.60	0.45	3.920

[a] from the Korea Thermophysical Property Data Bank or from the database of HYSYS

[b] molar volumes from Reid et al. [1], Nakanishi [18], Perry and Green [28], the Aldrich cataloge [53] and Cibulka et al. [54-59]

[c] some of the melting temperatures were taken from [53]

[d] radii of gyration of noble gases from Bosse and Reich [60]

[e] van der Waals parameters from [1, 61, 62]

[f] LSER parameters from [22,38]

Table 3
Numerical constants of Eq. (14)

k	C_{1k}	C_{2k}	C_{3k}	C_{4k}	C_{5k}	C_{6k}
n=1						
1	0.657728	-0.240632	0.075115	-0.060986	-0.310287	0.169494
2	-0.250986	0.201246	-0.671586	0.354609	1.285966	-0.008729
3	0.425222	0.124706	0.315845	-1.326663	-0.709235	0.013437
4	0.154399	-0.022536	-0.786000	-0.353124	1.014124	0.077913
5	-0.793954	0.008736	0.186054	2.344606	0.431023	-0.112510
6	-0.074194	0.012997	-0.001166	0.072078	0.039364	-0.010765
n=1/2						
1	0.876084	-0.134539	0.081922	-0.119188	-0.258646	0.079576
2	-0.250142	0.124614	-0.454201	0.226703	0.864954	0.034746
3	0.358917	0.124127	0.243279	-0.896910	-0.437587	-0.043534
4	0.023074	0.038244	-0.449969	-0.150081	0.650614	0.039465
5	-0.642833	-0.121353	-0.068082	1.604333	0.406097	0.028611
6	-0.067706	0.003552	-0.001375	0.066148	0.033067	-0.000959

Table 4
Average absolute deviations (%) of Eq. (14) and the other predictive equations

Solvent	Number of systems	NDP	Eq. (14) with n=1	Eq. (14) with n=1/2	Wilke-Chang Eq. (2)[a]	Kooijman Eq. (4)	Tyn-Calus Eq. (6)[b]	Nakanishi Eq. (9)	Hayduk-Minhas Eq (8)[b]	Hayduk-Minhas Eq. (3)
n-Pentane	2	2	8.31	11.76	16.77	3.49	14.57	9.31	21.91	28.45
n-Hexane	37	68	7.90	8.03	10.57	10.30	9.84	10.04	9.77	14.89
n-Heptane	14	19	9.39	11.38	16.55	13.46	14.57	11.80	16.72	21.07
n-Octane	23	27	7.14	9.55	9.84	12.90	11.36	13.11	11.33	17.82
n-Nonane	3	4	5.28	8.43	15.05	8.84	9.44	8.72	8.23	6.93
n-Decane	15	21	10.56	14.67	11.81	12.56	12.35	11.88	12.42	12.97
n-Dodecane	11	12	4.81	9.14	21.34	25.76	24.53	11.51	21.55	25.84
n-Tetradecane	25	27	14.55	14.87	20.12	33.33	29.52	11.32	21.86	18.87
n-Hexadecane	10	12	28.59	13.26	33.93	43.91	39.16	13.51	30.17	27.49
Cyclohexane	18	34	12.39	12.86	18.97	16.12	22.41	11.31	20.03	14.53
Methylcyclohexane	4	4	43.94	46.58	44.71	41.87	43.97	44.20	44.92	51.07
Benzene	21	46	11.07	11.65	13.89	12.10	17.54	15.05	17.51	13.80
Toluene	25	45	19.25	20.36	13.60	14.91	14.80	15.71	15.15	11.80
Isopropylbenzene	1	1	0.63	3.52	3.17	15.04	18.04	17.14	16.07	19.08
Diethyl ether	1	1	60.72	65.78	37.18	49.57	20.50	26.36	14.79	6.12
Acetone	46	64	11.94	11.97	15.95	10.87	8.59	14.66	10.78	12.51
Methyl ethyl ketone	3	3	24.88	29.06	12.22	14.40	5.12	17.57	3.43	3.42
Diethyl ketone	1	1	34.55	40.99	19.90	8.56	1.02	44.95	3.56	5.12

Solvent	Number of systems	NDP	Eq. (14) with n=1	Eq. (14) with n=1/2	Wilke-Chang Eq. (2)[a]	Kooijman Eq. (4)	Tyn-Calus Eq. (6)[b]	Nakanishi Eq. (9)	Hayduk-Minhas Eq (8)[b]	Hayduk-Minhas Eq. (3)
Methyl isobutyl ketone	3	3	22.03	26.96	38.50	29.73	18.94	28.79	21.72	19.72
Ethyl acetate	2	2	15.42	16.10	28.15	31.69	20.84	15.90	22.28	23.24
Butyl acetate	3	3	19.21	21.29	35.90	25.78	6.55	22.34	5.76	22.41
Ethyl benzoate	1	1	29.47	26.69	12.03	25.19	23.03	32.63	15.56	8.76
Acetonitrile	18	22	20.53	22.18	27.10	10.48	18.93	21.20	22.44	17.65
Nitrobenzene	3	3	19.91	22.84	25.20	46.32	39.16	30.72	33.96	24.68
Chloroform	17	19	6.65	6.74	33.56	19.19	20.42	21.66	17.43	18.95
Carbon tetrachloride	47	86	11.86	14.81	28.96	17.31	15.81	10.85	16.08	20.42
Bromoform	1	1	8.87	12.81	91.74	7.05	14.58	11.84	23.09	29.42
Chlorobenzene	7	9	8.07	14.81	5.45	12.85	14.01	12.57	13.51	12.43
Bromobenzene	1	1	3.41	4.98	20.15	5.79	10.25	21.75	5.55	3.52
Carbon disulfide	3	4	37.71	41.46	32.20	25.81	15.62	2.72	19.59	15.73
Water	51	133	7.82	8.18	10.86	16.10	12.51	10.60	11.99	10.96
Methanol	40	61	7.13	8.31	25.55	20.36	11.79	16.36	11.56	22.70
Ethanol	38	63	11.29	10.90	31.83	26.48	18.75	20.52	22.49	30.44
1-Propanol	8	14	26.94	26.01	64.62	42.97	28.69	51.46	34.36	59.20
2-Propanol	5	7	8.03	9.85	35.52	32.30	15.94	24.02	21.30	40.24
1-Butanol	14	14	23.57	20.52	42.41	47.60	24.10	34.26	29.93	45.23
Isobutanol	1	2	38.42	35.03	61.32	69.88	33.89	42.45	25.01	60.37
1-Pentanol	5	6	28.87	26.22	50.22	57.42	26.43	32.07	33.23	38.92
1-Hexanol	6	7	15.89	14.76	37.87	38.92	47.36	24.79	72.31	29.11

Solvent	Number of systems	NDP	Eq. (14) with n=1	Eq. (14) with n=1/2	Wilke-Chang Eq. (2)[a]	Kooijman Eq. (4)	Tyn-Calus Eq. (6)[b]	Nakanishi Eq. (9)	Hayduk-Minhas Eq (8)[b]	Hayduk-Minhas Eq. (3)
1-Heptanol	7	9	21.22	21.62	47.01	56.19	34.31	28.66	53.09	35.08
1-Octanol	23	42	12.50	12.00	51.10	55.51	28.15	32.91	50.42	43.26
Aniline	3	3	16.86	22.35	35.32	35.45	37.70	34.45	27.97	8.61
Acetic acid	6	8	11.77	9.89	19.29	13.40	12.58	21.52	14.60	28.03
Overall	550	914	12.23	12.86	22.65	20.97	16.93	16.33	18.52	20.27

[a] The association factor for other alcohols than methanol has been taken as 1.5.

[b] The parachor has been calculated with Eq. (7).

Appendix A. Supplementary data

Table

Diffusion coefficients of several binary systems at 298.15 K

Solvent	Solute	$10^9 D_{AB}$	Reference
n-pentane	methane	11.664	Interpolated from [23]
	n-pentane	5.535	[24]
n-hexane	methane	8.640	[5]
		8.730	[25]
	ethane	5.790	[14]
	propane	4.870	[26]
	n-pentane	4.590	[27]
	n-hexane	4.066	[28]
		4.233	[29]
		4.150	[30]
		4.210	[30]
		4.210	[30]
		4.160	[30]
	n-heptane	3.780	[27]
	n-octane	3.470	[27]
	n-decane	3.020	[27]
		4.630	[15]
	n-dodecane	2.740	[31]
		2.715	[32]
	n-hexadecane	2.210	[33]
		2.230	[2]
	n-octadecane	2.010	[27]
	2-methylbutane	4.400	[5]
	2,2-dimethylbutane	3.630	[5]
	2,2,4-trimethylpentane	3.380	[5]
	ethylene	7.820	[34]
	cyclohexane	3.973	[29]
		4.140	[35]
		3.770	[27]
		3.690	[2]
	cyclooctane	3.380	[2]
	benzene	4.610	Interpolated from [36]
		4.758	[37]
		4.790	[35]
		4.640	[5]
		4.680	[2]
		4.885	[29]
		4.711	[38]
		4.760	[38]
	toluene	4.377	[38]
		4.335	[39]
		4.210	[13]
	anthracene	3.020	[17]

Solvent	Solute	$10^9 D_{AB}$	Reference
		3.160	[17]
n-hexane	pyrene	2.800	[17]
		2.930	[17]
	acetone	4.860	[35]
	acetonitrile	6.100	[38]
		6.130	[38]
	nitrobenzene	3.890	Interpolated from [40]
	N, *N*-dimethylformamide	5.300	[2]
	carbon tetrachloride	3.890	[25]
		3.866	[39]
		3.840	[2]
		3.860	[31]
	chloroform	4.440	[2]
	1,2-dicloroethane	4.640	[2]
	bromobenzene	3.860	[2]
	argon	8.500	[25]
	krypton	6.300	[25]
	xenon	5.440	[25]
	carbon dioxide	8.200	[41]
	carbon disulfide	5.910	[2]
		5.840	[38]
		5.928	[38]
		5.962	[38]
		5.903	[38]
	water	9.530	[2]
	methanol	9.730	[2]
	ethanol	5.870	[2]
n-heptane	methane	7.520	[5]
	ethane	5.440	[14]
	propane	4.400	[26]
	n-heptane	2.956	Interpolated from [24]
		3.136	[42]
		3.120	[15]
	n-decane	2.540	[27]
		3.080	[15]
	n-dodecane	2.190	[27]
	n-tetradecane	1.940	[27]
	n-hexadecane	1.780	[31]
	benzene	3.915	[43]
		3.864	[37]
	toluene	3.720	[13]
	carbon tetrachloride	3.170	[13]
	carbon monoxide	8.120	[44]
	carbon dioxide	6.890	[41]
		6.030	[45]
	hydrogen	24.000	[44]
n-octane	methane	6.490	[5]

Solvent	Solute	$10^9 D_{AB}$	Reference
		6.080	[46]
n-octane	ethane	4.570	[14]
	propane	3.830	[26]
	n-heptane	2.500	[15]
	n-decane	2.400	[15]
	n-dodecane	1.718	[47]
	n-tetradecane	1.630	[27]
	n-hexadecane	1.426	[32]
	n-octadecane	1.200	[47]
	propene	3.410	[48]
		3.420	[49]
	methylcyclohexane	2.302	[50]
	anthracene	2.040	[17]
		2.010	[17]
	cyclohexanone	2.200	[50]
	carbon tetrachloride	2.558	[51]
		2.560	[46]
	argon	6.680	[46]
	krypton	5.000	[46]
	xenon	4.060	[46]
	methanol	4.790	[52], at 300 K
	ethanol	3.540	[52], at 300 K
	1-propanol	3.040	[52], at 300 K
	1-pentanol	2.580	[52], at 300 K
	1-heptanol	2.170	[52], at 300 K
	1-decanol	1.830	[52], at 300 K
n-nonane	*n*-heptane	2.020	[15]
	n-nonane	1.725	Interpolated from [42]
		1.642	Interpolated from [53]
	n-decane	1.900	[15]
n-decane	methane	5.397	Interpolated from [54]
		4.380	[46]
	n-heptane	1.730	[27]
		1.610	[15]
	n-decane	1.385	Interpolated from [42]
		1.550	[15]
		1.310	[53]
	n-hexadecane	0.950	[32]
	neopentane	1.710	[25]
	cyclohexane	1.760	[7]
	toluene	2.090	[13]
	cyclohexanone	1.670	[7]
	carbon tetrachloride	1.710	[51]
		1.720	[3]
		1.700	[46]
	1,1,1-tricloroethane	1.780	[3]
	tert-butylchloride	1.650	[3]

Solvent	Solute	$10^9 D_{AB}$	Reference
n-decane	argon	4.870	[46]
	krypton	3.510	[46]
	xenon	2.860	[46]
	cyclohexanol	1.640	[7]
n-dodecane	methane	3.940	[5]
	ethane	2.730	[14]
	n-hexane	1.420	[31]
		1.395	[32]
	n-heptane	1.300	[27]
	n-octane	1.136	[47]
	n-dodecane	0.870	Interpolated from [42]
	n-hexadecane	0.670	[57]
	n-octadecane	0.594	[47]
	ethylene	3.110	[34]
	toluene	1.380	[13]
	carbon tetrachloride	1.229	[51]
n-tetradecane	methane	2.780	[46]
	n-heptane	0.930	[27]
	n-octane	0.850	[27]
	n-tetradecane	0.581	Interpolated from [42]
	neopentane	0.842	[25]
	benzene	1.180	[6]
	toluene	1.070	[6]
		1.020	[13]
	o-xylene	0.892	[4]
	m-xylene	0.943	[4]
	p-xylene	1.020	[4]
	ethylbenzene	0.953	[6]
	propylbenzene	0.871	[6]
	naphthalene	0.889	[6]
	biphenyl	0.792	[6]
		0.790	[17]
	pyridine	1.190	[55]
	carbon tetrachloride	0.897	[46]
	chlorobenzene	1.060	[6]
	o-dichlorobenzene	0.888	[4]
	m-dichlorobenzene	0.936	[4]
	p-dichlorobenzene	1.000	[4]
	argon	3.400	[46]
	krypton	2.370	[46]
	xenon	1.720	[46]
	carbon dioxide	2.950	[56]
	aniline	0.994	[55]
n-hexadecane	methane	2.660	[5]
	ethane	1.950	[14]
	propane	1.480	[26]
	n-hexane	0.850	[33]

Solvent	Solute	$10^9 D_{AB}$	Reference
n-hexadecane	*n*-heptane	0.740	[31]
	n-decane	0.570	[32]
	n-dodecane	0.490	[57]
	n-hexadecane	0.378	[58]
		0.425	Interpolated from [42]
	anthracene	0.535	[17]
		0.540	[17]
	carbon dioxide	2.210	[14]
isooctane	ethano	4.650	[59]
	ethylene	5.080	[59]
	carbon dioxide	6.340	[59]
cyclohexane	methane	4.110	[60]
	ethane	2.920	[36]
	n-hexane	1.641	[29]
		1.800	[35]
	ethylene	3.200	[36]
	cyclohexane	1.340	[61]
		1.447	Interpolated from [62]
		1.450	[63]
		1.394	Interpolated from [64]
		1.441	[65]
		1.380	[66]
	benzene	1.836	[67]
		1.896	[43]
		1.876	[68]
		1.880	[69]
		1.950	[35]
	toluene	1.728	[67]
		1.569	[43]
	p-xylene	1.645	[67]
	1,3,5-trimethylbenzene	1.400	[67]
	naphthalene	1.452	[67]
	phenanthrene	1.199	[67]
	acetone	2.220	[70]
		2.080	[35]
	carbon tetrachloride	1.486	[43]
		1.484	[71]
		1.490	[1]
		1.490	[13]
		1.490	[60]
	argon	4.710	[60]
	krypton	3.570	[60]
	xenon	3.030	[60]
	carbon disulfide	2.200	[72]
	water	3.400	[10]
methylcyclohexane	*n*-octane	1.611	[50]
	methylcyclohexane	1.915	[73]

Solvent	Solute	$10^9 D_{AB}$	Reference
	toluene	1.650	[74]
methylcyclohexane	1-heptanol	0.618	[50]
benzene	methane	4.860	[25]
	n-hexane	2.312	[37]
		2.540	[35]
		2.355	[29]
	n-heptane	1.785	[43]
		2.130	[37]
	cyclohexane	2.090	[43]
		2.090	[69]
		2.170	[35]
	benzene	2.210	[75]
		2.210	[75]
		2.210	[75]
		2.180	[75]
		2.207	[76]
		2.270	[77]
		2.189	Interpolated from [42]
		2.200	Interpolated from [64]
		2.202	[29]
		2.227	[65]
		2.210	[78]
	toluene	1.820	[1]
	diethyl ether	2.730	[13]
	acetone	2.750	[69]
		2.780	[35]
	chloroform	2.245	[1]
		2.500	[13]
	carbon tetrachloride	1.950	[25]
		1.920	[79]
		2.000	[12]
		2.040	[13]
	chlorobenzene	2.120	[79]
		2.660	[13]
	bromobenzene	2.300	[13]
	krypton	4.320	[25]
	xenon	3.570	[25]
	carbon dioxide	4.460	[41]
		4.050	[41]
		3.850	[80]
	water	6.310	[10]
	methanol	4.275	[81, 82]
		3.820	[83]
	ethanol	3.618	Interpolated from [81, 82]
		3.300	[83]
	3-pentanol	1.680	[13]
	aniline	1.960	[84]

Solvent	Solute	$10^9 D_{AB}$	Reference
	acetic acid	2.110	[13]
toluene	*n*-hexane	2.479	[39]
		2.390	[2]
	propene	2.200	[85]
		2.430	[85]
		2.180	[85]
	cyclohexane	2.420	[43]
		2.100	[2]
	methylcyclohexane	2.210	[74]
	cyclooctane	1.940	[2]
	benzene	2.545	[1]
		2.400	[2]
	toluene	2.280	Interpolated from [86]
		2.323	[87]
		2.240	[88]
		2.210	[88]
		2.290	[88]
	acetone	2.940	[2]
	acetonitrile	3.170	[2]
	N, *N*-dimethylformamide	2.430	[2]
	chloroform	2.520	[2]
	carbon tetrachloride	2.143	[39]
		2.190	[89]
		2.170	[2]
	1,2-dichloroethane	2.490	[2]
	chlorobenzene	2.240	[79]
	bromobenzene	2.050	[2]
	nitrogen	5.800	[90]
		6.190	[85]
		6.070	[85]
	nitrous oxide	5.020	[90]
	carbon monoxide	5.700	[90]
	carbon dioxide	4.890	[90]
		4.600	[56]
		4.460	[41]
		4.330	[41]
		4.140	[85]
		3.910	[85]
	carbon disulfide	3.240	[2]
	water	6.190	[2]
		6.070	[10]
		6.120	[10]
	methanol	3.990	[2]
	ethanol	3.110	[2]
	aniline	2.100	[74]
	acetic acid	2.265	[89]

Solvent	Solute	$10^9 D_{AB}$	Reference
isopropylbenzene	acetone	2.483	Interpolated from [91]
diethyl ether	chloroform	4.510	[92]
acetone	methane	7.250	[25]
	n-hexane	4.030	[35]
	propene	6.190	[48]
	cyclohexane	4.060	[70]
		3.850	[35]
	benzene	4.120	[69]
		4.280	[35]
		4.070	[6]
	toluene	3.750	[6]
	o-xylene	3.390	[4]
	m-xylene	3.420	[4]
	p-xylene	3.520	[4]
	1,2,4-trimethylbenzene	3.160	[4]
	1,3,5-trimethylbenzene	3.160	[4]
	ethylbenzene	3.450	[6]
	propylbenzene	3.240	[6]
	isopropylbenzene	3.023	Interpolated from [91]
	naphthalene	3.250	[6]
	biphenyl	2.890	[6]
	anthracene	2.850	[6]
	anisole	3.470	[93]
	acetone	4.653	Interpolated from [42]
		4.300	Interpolated from [86]
		4.137	Interpolated from [94]
		4.874	Interpolated from [66]
		4.570	[78]
	acetophenone	3.230	[93]
	pyridine	3.940	[55]
	o-nitrotoluene	3.110	[22]
	m-nitrotoluene	3.140	[22]
	chloroform	3.620	[95]
		3.620	[96]
	carbon tetrachloride	3.630	[25]
		3.480	[1]
		4.060	[35]
		3.610	[3]
	bromoform	3.240	[97]
		2.900	[13]
	1,1,1-trichloroethane	3.650	[3]
	tert-butylcloride	3.620	[3]
	chlorobenzene	3.710	[6]
	o-dichlorobenzene	3.350	[4]
		3.273	Interpolated from [91]
	m-dichlorobenzene	3.380	[4]
	p-dichlorobenzene	3.460	[4]

Solvent	Solute	$10^9 D_{AB}$	Reference
acetone	krypton	6.140	[25]
	xenon	5.180	[25]
	carbon dioxide	6.080	[41]
	water	5.220	[95]
		5.500	[69]
		4.560	[89]
		5.260	[10]
	phenol	2.970	[55]
		2.930	[93]
	p-chlorophenol	2.660	[93]
	o-methylphenol	2.780	[22]
	p-cresol	2.740	[55]
		2.720	[93]
	2,5-dimethylphenol	2.610	[22]
	2,6-dimethylphenol	2.750	[22]
	aniline	3.170	[55]
	p-chloroaniline	2.920	[55]
	p-toluidine	2.940	[55]
	acetic acid	3.309	[89]
methyl-ethyl-ketone	chloroform	2.860	[97]
	carbon tetrachloride	3.007	[98]
	carbon dioxide	4.810	[41]
diethyl ketone	carbon dioxide	4.670	[41]
methyl isobutyl ketone	chloroform	2.100	[97]
	carbon dioxide	4.400	[56]
	acetic acid	1.929	Interpolated from [91]
cyclohexanone	*n*-octane	0.741	[50]
	cyclohexanone	0.631	[61]
	1-heptanol	0.576	[50]
ethyl acetate	propene	4.980	[48]
	chloroform	2.530	[97]
butyl acetate	chloroform	1.960	[97]
	water	2.920	[10]
	acetic acid	1.687	[91]
ethyl benzoate	ethy acetate	0.940	[13]
acetonitrile	ethane	5.760	[59]
	n-hexane	3.700	[2]
	ethylene	6.200	[59]
	cyclohexane	3.230	[2]
		3.740	[7]
	benzene	3.810	[2]
	toluene	3.380	[2]
	cyclohexanone	3.160	[7]
	acetonitrile	4.370	[78]
		4.310	[99]
		4.350	[99]
	N, N-dimethylformamide	3.410	[2]

Solvent	Solute	$10^9 D_{AB}$	Reference
	chloroform	3.390	[2]
acetonitrile	carbon tetrachloride	3.320	[25]
		3.450	[2]
	1,2-dichloroethane	3.460	[2]
	bromobenzene	3.140	[2]
	carbon disulfide	4.910	[100]
	water	5.780	[2]
	methanol	4.900	[100]
	ethanol	3.980	[2]
	cyclohexanol	2.960	[7]
nitrobenzene	*n*-hexane	0.907	Interpolated from [40]
	benzene	1.240	Extrapolated from [29]
	water	2.800	[10]
N,*N*-dimethylformamide	propene	1.880	[48]
	N, *N*-dimethylformamide	1.610	[101]
		1.630	[78]
		1.640	[102]
	water	1.810	[10]
		1.719	[103]
		2.115	Interpolated from [104]
chloroform	benzene	2.885	[1]
	toluene	2.010	[105], at 296.6 K
	ethylbenzene	1.800	[105], at 296.6 K
	propylbenzene	1.580	[105], at 296.6 K
	isopropylbenzene	1.660	[105], at 296.6 K
	butylbenzene	1.460	[105], at 296.6 K
	isobutylbenzene	1.500	[105], at 296.6 K
	tert-butylbenzene	1.580	[105], at 296.6 K
	sec-butylbenzene	1.540	[105], at 296.6 K
	diethyl ether	2.147	[92]
	acetone	2.330	[95]
		2.410	[96]
	methyl ethyl ketone	2.130	[97]
	methyl isobutyl ketone	1.890	[97]
	ethyl acetate	2.020	[97]
	butyl acetate	1.710	[97]
	chloroform	2.420	Interpolated from [106]
		2.555	Interpolated from [107]
	phenol	2.000	[13]
carbon tetrachloride	methane	2.780	[108]
		3.080	[25]
	ethane	2.360	[109]
	n-pentane	1.560	[110]
	n-hexane	1.468	[39]
		1.620	[35]
		1.500	[110]
		1.480	[31]

Solvent	Solute	$10^9 D_{AB}$	Reference
carbon tetrachloride	*n*-heptane	1.330	[110]
	n-octane	1.254	[51]
		1.260	[110]
	n-decane	1.074	[51]
		1.080	[110]
	n-dodecane	0.959	[51]
		0.960	[110]
		0.954	[5]
	n-hexadecane	0.760	[110]
		0.780	[5]
	n-octadecane	0.690	[110]
	n-eicosane	0.660	[110]
		0.664	[5]
	n-docosane	0.620	[5]
	2-methylbutane	1.490	[5]
	2,2-dimethylbutane	1.250	[5]
	isooctane	1.130	[5]
	cyclohexane	1.275	[43]
		1.283	[71]
		1.260	[1]
	benzene	1.370	[79]
		1.530	[13]
	toluene	1.479	[39]
		1.400	[5]
	1,3,5-trimethylbenzene	1.190	[5]
	naphthalene	1.200	[5]
	biphenyl	1.070	[5]
	biphenyl methane	0.985	[5]
	phenanthrene	1.030	[5]
	anthracene	1.030	[5]
	tetrahydrofurane	1.470	[5]
	acetone	1.690	[1]
		1.700	[35]
	methyl ethyl ketone	1.552	[98]
	nitrobenzene	1.000	[13]
	dimethyl acetamide	1.230	[5]
	carbon tetrafluoride	2.040	[108]
	chloroform	1.505	[111]
	carbon tetrachloride	1.300	[75]
		1.370	[75]
		1.296	[76]
		1.301	[64]
		1.412	[112]
	argon	3.630	[108]
		3.710	[113]
		3.790	[25]
		3.110	[114]

Solvent	Solute	$10^9 D_{AB}$	Reference
		3.270	[114]
carbon tetrachloride	argon	3.460	[114]
	krypton	2.860	[25]
	xenon	2.500	[25]
	nitrogen	3.420	[108]
		3.630	[113]
		3.640	[114]
		3.590	[114]
		3.560	[114]
	oxygen	3.820	[115]
		3.710	[116]
		3.400	[114]
		3.590	[114]
		3.790	[114]
	carbon dioxide	3.200	[41]
		2.950	[41]
		3.170	[80]
	sulfur hexafluoride	1.710	[5]
	hydrogen	9.750	[108]
	water	4.120	[117]
		4.070	[117]
	methanol	2.446	[118]
		2.610	[5]
	ethanol	1.901	[118]
		1.950	[5]
	phenol	1.370	[5]
	benzyl alcohol	1.280	[5]
	aniline	1.580	[84]
	acetic acid	1.365	[98]
		1.490	[89]
		1.420	[5]
bromoform	acetone	0.712	[97]
chlorobenzene	propane	2.770	[26]
	propene	2.410	[48]
	benzene	1.870	[37]
	toluene	1.684	[79]
	chlorobenzene	1.744	Interpolated from [42]
		1.865	Interpolated from [94]
	bromobenzene	1.658	[79]
	carbon dioxide	3.690	[85]
		3.930	[85]
o-dichlorobenzene	acetone	1.293	Interpolated from [91]
	water	3.330	[10]
bromobenzene	chlorobenzene	1.267	[79]
carbon disulfide	cyclohexane	2.850	[72]
	carbon disulfide	4.200	[119]

Solvent	Solute	$10^9 D_{AB}$	Reference
		4.260	[81]
carbon disulfide	ethanol	2.288	[110]
water	methane	1.885	Interpolated from [120]
		1.713	Interpolated from [121]
		1.990	[122]
	ethane	1.710	[123]
		1.880	[123]
		1.523	Interpolated from [120]
		1.385	Interpolated from [121]
		1.530	[122]
	propane	1.212	Interpolated from [120]
		1.170	Interpolated from [121]
		1.270	[122]
	n-butane	0.963	Interpolated from [120]
		1.065	Interpolated from [121]
		0.970	[122]
	n-pentane	1.000	Interpolated from [121]
	cyclopentane	1.050	Interpolated from [124]
	methylcyclopentane	0.968	Interpolated from [124]
	cyclohexane	0.958	Interpolated from [124]
	benzene	1.100	[18]
		1.190	Interpolated from [19]
		1.165	Interpolated from [124]
		1.130	[125]
		1.060	[125]
	toluene	0.973	Interpolated from [124]
		0.930	[125]
	ethylbenzene	0.933	Interpolated from [124]
	butylbenzene	0.780	[19]
	naphthalene	0.937	[19]
	1-ethylnaphthalene	0.780	[19]
	biphenyl	0.833	[19]
	diethyl ether	0.850	[13]
	tetrahydrofurane	1.090	[9]
	dioxane	1.110	[9]
	acetone	1.300	[95]
		1.280	[69]
		1.170	[125]
	ethyl acetate	1.375	Interpolated from [126]
	acetonitrile	1.640	[2]
	N, *N*-dimethylformamide	1.000	[2]
		1.011	[103]
	chlorobenzene	1.040	[125]
		1.000	[125]
		0.980	[125]
	o-dichlorobenzene	0.940	[125]
		0.890	[125]

Solvent	Solute	$10^9 D_{AB}$	Reference
		0.870	[125]
water	*p*-dichlorobenzene	0.990	[125]
		0.930	[125]
	bromobenzene	1.030	[125]
		0.990	[125]
		0.960	[125]
	xenon	0.827	[127]
		0.810	[128]
	nitrous oxide	1.880	[129]
		1.880	[130]
		1.800	[130]
		1.780	[130]
		1.920	[130]
		1.860	[131]
		1.690	[132]
	carbon dioxide	1.910	[133]
		1.946	[134]
		1.900	[134]
		1.850	[134]
		1.820	[134]
		1.870	[134]
		1.900	[134]
		1.920	[134]
		2.050	[134]
		2.000	[134]
		1.970	[135]
		1.940	[136]
		1.940	[129]
		1.920	[137]
		1.950	[138]
		1.890	[122]
		1.980	[131]
		1.930	[41]
		1.940	[41]
		1.950	[139]
		1.960	[139]
	water	2.300	[140]
		2.300	[141]
		2.299	[142]
		2.130	[143]
		2.230	[144]
		2.525	[24]
		2.250	[145]
	methanol	1.709	Interpolated from [146]
		1.540	[147]

Solvent	Solute	$10^9 D_{AB}$	Reference
		1.563	[148]
water	methanol	1.605	[104]
		1.560	[2]
	ethanol	1.240	[20]
		1.268	Interpolated from [146]
		1.220	[147]
		1.240	[1]
		1.220	[2]
	1-propanol	1.050	[20]
		1.157	Interpolated from [146]
		1.050	[147]
		0.990	[2]
		1.150	Extrapolated from [149]
	isopropanol	1.157	Interpolated from [146]
		1.020	[147]
	1-butanol	0.933	[20]
		1.007	Interpolated from [146]
		0.960	[147]
		0.970	[150]
	2-butanol	0.940	[147]
	isobutanol	0.950	[147]
	tert-butanol	0.985	Interpolated from [146]
		0.874	[20]
		0.870	[147]
	1-pentanol	0.920	[151]
		0.880	[147]
	2-pentanol	0.911	[151]
	3-pentanol	0.899	[151]
	2-methyl-1-butanol	0.920	[151]
	2-methyl-2-butanol	0.873	[151]
	3-methyl-1-butanol	0.903	[151]
		1.000	[13]
	1-hexanol	0.830	[147]
	1-heptanol	0.800	[147]
	acetic acid	1.250	[152]
		1.271	[152]
		1.210	[152]
		1.295	[153]
		1.101	Interpolated from [91]
	propionic acid	1.009	[152]
	butyric acid	0.918	[152]
	valeryc acid	0.817	[152]
	caproic acid	0.784	[152]
methanol	methane	5.810	[16]
	ethane	4.380	[59]
	ethylene	4.710	[59]
	cyclohexane	2.500	[7]

Solvent	Solute	$10^9 D_{AB}$	Reference
	benzene	2.813	[81, 82]
methanol	benzene	2.610	[21]
		2.660	[83]
	toluene	2.560	[11]
		2.420	[21]
	1,3,5-trimethylbenzene	2.020	[21]
	ethylbenzene	2.230	[21]
	propylbenzene	2.060	[21]
	1-methylnaphthalene	1.900	[21]
	biphenyl	1.890	[11]
		1.850	[21]
	acetophenone	2.070	[21]
	cyclohexanone	2.170	[7]
	benzaldehyde	2.170	[21]
	pyridine	2.070	[55]
	acetonitrile	3.430	[100]
	benzonitrile	2.250	[21]
	nitrobenzene	2.280	[21]
	o-nitrotoluene	2.070	[21]
	carbon tetrachloride	2.250	[16]
		2.248	[118]
		2.270	[3]
		2.300	[13]
	bromoform	2.200	[13]
	1,1,1-trichloroethane	2.280	[3]
	tert-butylchloride	2.270	[3]
	chlorobenzene	2.400	[21]
	argon	6.430	[16]
	krypton	5.100	[16]
	xenon	3.970	[16]
	carbon dioxide	5.130	[135]
		8.020	[135]
		5.550	[59]
		4.540	[80]
		4.950	[41]
		8.370	[139]
	water	2.190	[148]
		2.115	Interpolated from [104]
	methanol	2.340	[75]
		2.210	[75]
		2.370	[75]
		2.270	[154]
		2.410	[78]
		2.485	[78]
		2.440	[145]
		2.420	[155]

Solvent	Solute	$10^9 D_{AB}$	Reference
		2.410	[155]
methanol	cyclohexanol	1.730	[7]
	phenol	1.690	[55]
	p-chlorophenol	1.580	[21]
	o-cresol	1.610	[21]
	p-cresol	1.590	[55]
	ammonia	2.337	Interpolated from [135]
	aniline	1.940	[55]
	p-chloroaniline	1.780	[55]
	p-toluidine	1.790	[55]
	m-toluidine	1.800	[21]
ethanol	cyclohexane	1.530	[7]
	benzene	2.455	Interpolated from [81, 82]
		1.790	[6]
		1.970	[83]
	toluene	1.620	[6]
	o-xylene	1.400	[4]
	m-xylene	1.440	[4]
	p-xylene	1.540	[4]
	1,3,5-trimethylbenzene	1.320	[8]
	ethylbenzene	1.450	[6]
	propylbenzene	1.320	[6]
	naphthalene	1.320	[6]
	biphenyl	1.160	[11]
		1.190	[6]
		1.200	[8]
	anthracene	1.040	[6]
	cyclohexanone	1.340	[7]
	pyridine	1.200	[55]
	pyrazine	1.540	[8]
	nitrobenzene	1.440	[8]
	chloroform	1.380	[13]
	carbon tetrachloride	1.500	[25]
		1.500	[1]
		1.470	[3]
	bromoform	1.080	[13]
	1,1,1-trichloroethane	1.470	[3]
	tert-butylchloride	1.460	[3]
	chlorobenzene	1.610	[6]
	o-dichlorobenzene	1.370	[4]
	m-dichlorobenzene	1.430	[4]
	p-dichlorobenzene	1.540	[4]
	nitrous oxide	4.260	[90]
	carbon dioxide	4.110	[90]
		4.050	[41]
		3.660	[41]

Solvent	Solute	$10^9 D_{AB}$	Reference
		3.420	[45]
ethanol	carbon dioxide	4.500	[136]
		3.860	[80]
		4.000	[13]
		3.880	[139]
	carbon disulfide	2.528	Interpolated from [81, 82]
	water	1.130	[1]
		1.220	[10]
		1.180	[10]
	ethanol	1.056	[156]
		1.160	[157]
		1.020	[75]
		1.050	[75]
		1.000	[75]
		1.020	[75]
		1.010	[154]
		1.070	[78]
		1.423	Interpolated from [86]
		1.160	[145]
	cyclopentanol	0.920	[7]
	cyclohexanol	0.865	[7]
	phenol	0.890	[13]
		0.878	[8]
	aniline	1.190	[55]
	o-nitroaniline	1.050	[8]
	m-nitroaniline	0.945	[8]
	p-nitroaniline	0.846	[8]
	acetic acid	1.032	[153]
1-propanol	benzene	1.280	[11]
	toluene	1.350	[11]
	biphenyl	0.727	[11]
	bromoform	0.940	[13]
	carbon dioxide	3.170	[41]
		3.060	[80]
		2.730	[139]
	hydrogen	11.900	[158]
		12.840	[158]
	water	0.480	Extrapolated from [149]
	1-propanol	0.590	[156]
		0.600	[159]
		0.646	[154]
		0.590	[145]
2-propanol	methane	3.180	[25]
	carbon tetrachloride	0.936	[25]
	krypton	2.530	[25]
	xenon	1.760	[25]

Solvent	Solute	$10^9 D_{AB}$	Reference
	2-propanol	0.600	[159]
2-propanol	2-propanol	0.649	[154]
		0.582	[145]
1-butanol	methane	2.660	[16]
	propane	1.570	[26]
	ethylene	2.310	[34]
	propene	1.340	[48]
	cyclohexane	0.659	[160]
	methylcyclohexane	0.710	[160]
	benzene	0.988	[11]
	biphenyl	0.627	[11]
	carbon tetrachloride	0.843	[16]
	argon	3.310	[16]
	krypton	2.190	[16]
	xenon	1.620	[16]
	water	0.550	[150]
	1-butanol	0.504	[154]
isobutanol	carbon dioxide	2.130	[41]
		2.200	[45]
1-pentanol	cyclohexane	0.584	[160]
	methylcyclohexane	0.638	[160]
	benzene	0.985	[11]
	biphenyl	0.571	[11]
	carbon dioxide	2.160	[41]
		1.910	[45]
1-hexanol	*n*-heptane	0.480	[15]
	n-decane	0.480	[15]
	cyclohexane	0.475	[7]
		0.574	[160]
	methylcyclohexane	0.616	[160]
	cyclohexanone	0.392	[7]
	cyclohexanol	0.224	[7]
1-heptanol	*n*-heptane	0.430	[15]
	n-decane	0.370	[15]
	cyclohexane	0.511	[160]
	methylcyclohexane	0.470	[50]
		0.573	[160]
	benzene	0.640	[11]
	cyclohexanone	0.335	[50]
	carbon dioxide	1.660	[41]
		1.800	[41]
1-octanol	methane	1.450	[52]
		1.450	[16]
	ethane	0.912	[52]
	propane	0.661	[52]
	n-pentane	0.522	[52]
	n-heptane	0.448	[52]

Solvent	Solute	$10^9 D_{AB}$	Reference
	n-decane	0.354	[52]
1-octanol	cyclohexane	0.464	[160]
	methylcyclohexane	0.499	[160]
	benzene	0.470	[161]
		0.501	[161]
		0.484	[161]
		0.507	[161]
	toluene	0.436	[161]
		0.442	[161]
		0.459	[161]
		0.461	[161]
	carbon tetrachloride	0.381	[16]
	chlorobenzene	0.422	[161]
		0.428	[161]
		0.449	[161]
		0.444	[161]
		0.445	[161]
	o-dichlorobenzene	0.316	[161]
		0.335	[161]
		0.344	[161]
		0.349	[161]
		0.354	[161]
	p-dichlorobenzene	0.387	[161]
		0.411	[161]
	bromobenzene	0.401	[161]
		0.407	[161]
	argon	1.860	[16]
	krypton	1.190	[16]
	xenon	0.845	[16]
	carbon dioxide	1.500	[41]
		1.460	[41]
		1.460	[56]
	methanol	0.212	[52]
	ethanol	0.189	[52]
	propanol	0.175	[52]
	1-pentanol	0.155	[52]
aniline	benzene	0.540	[84]
	toluene	0.478	[74]
	carbon tetrachloride	0.520	[84]
acetic acid	propene	1.760	[48]
	methyl isobutyl ketone	0.984	Interpolated from [91]
	butyl acetate	1.040	Interpolated from [91]
	carbon tetrachloride	1.280	[98]
acetic acid	water	1.118	Interpolated from [91]
	acetic acid	1.058	[42]
		1.170	Interpolated from [86]
		0.993	[64]

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