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New tracer diffusion correlation for real systems over wide ranges of temperature and density

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ABSTRACT

In this work a new model for tracer diffusivities (D_{12}) of real systems is proposed. It is applicable for gases, liquids and supercritical fluids over wide ranges of temperature and density. It was derived on the basis of a very accurate hard sphere expression, following a systematic derivation whereby the softness of repulsive interactions and the contribution of attractive forces were taken into account by means of effective diameters and by coupling an attractive exponential term. The model is explicit and requires only temperature, density, and one diffusive parameter. The validation was accomplished with the largest database ever compiled – 314 binary systems and 5421 data points – giving rise to an average deviation of only 4.40%. Finally it must be emphasized the reliable estimation capability of the new model, i.e. its capacity to predict D_{12} at temperatures and densities far away from the conditions of the experimental data utilized to fit its parameter.

1. Introduction

Diffusion is a microscopic level phenomenon that results from particles motion and interaction. The proportionality constant between particles flux and concentration gradient defines the diffusion coefficient [1,2], which may be experimentally measured or estimated by computer simulations or macroscopic models. Typically, tracer diffusion coefficients (D_{12}) are measured by the chromatographic-peak-broadening technique, based on the Taylor–Aris dispersion phenomenon, or by the geometric method [3,4]. With relation to computer simulations, diffusion coefficients, as well as other transport coefficients, may be calculated from equilibrium correlation functions, by observing Green–Kubo formulas or the associated Einstein relations, or going back to first principles and conducting suitable non-equilibrium simulations [2,5].

The tracer diffusion coefficients are fundamental properties in research and industry. The lack of experimental data and reliable/accurate equations to estimate them in compressed and condensed phases constitute basic shortcomings. For most concentrated liquid mixtures, binary and effective diffusivities can be estimated on the basis of the tracer coefficients of the implied components using the Darken [6], the Vignes [7], or any other of the equations reviewed by Pertler et al. [8].

Up till now it is not yet possible to give a rigorous theoretical interpretation of the transport properties of dense fluids, because of the many-body interactions involved and the pair potential energy functions are only known for simple molecules. However, the repulsive interaction in condensed phases plays a major role in their properties, which means that an accurate model for hard spheres (HS) can be used as a first approximation for the major excluded volume and packing effects of real substances. In fact, it has been found that for the liquid viscosity and diffusivity the contribution of the hard sphere term is up to about 70% [2], which evidences its predominance over the attractive contribution. Nonetheless, for proper application of the Hard Sphere (HS) theory, it is necessary to take into account corrections for correlated motions dominant at intermediate and high densities, which may be assessed by computer simulations, specifically by equilibrium and/or non-equilibrium molecular dynamics [1,2,9].

The main theories for transport properties of dense fluids are the milestone Enskog theory of the HS fluid, the modified Enskog theory applicable to real fluids, the effective hard sphere diameter method, the free-volume approaches (e.g., Dymond, Cohen–Turnbull, Macedo–Litovitz, Chung), the van der Waals and rough hard sphere theories, the hydrodynamic theories based on the Stokes–Einstein equation, the Eyring activated-state theory, and the excess entropy scaling laws which are receiving much attention recently [1,2,10–21].

In this work it is presented a new tracer diffusion coefficients model for real systems derived on the basis of the HS model fluid. The softness of repulsive interactions is taken into account by means of the effective hard sphere diameter method, and the

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Nomenclature

AARD	Average absolute relative deviation, $AARD = \left(\frac{100}{NDP}\right) \times \sum_{i-1}^{NDP} \left\lvert (D^{calc}_{12,Real} - D^{exp}_{12,Real})/D^{exp}_{12,Real} \right\rvert_i$
B	Parameter in Eq. (27)
D	Diffusion coefficient, cm^2/s
F	Correction factor of HS system
$g(\sigma)$	Radial distribution function at contact
HS	Hard sphere fluid
k_B	Boltzmann constant, 1.380658×10^{-16} erg/K
m	Mass of a molecule, g
M	Molecular weight
MD	Molecular Dynamics
NDP	Number of data points
NS	Number of systems
N_a	Avogadro constant, 6.0221367×10^{23} mol^{-1}
P	Pressure, bar
R_g	Gas constant, 8.31541×10^7 erg/mol K
T	Temperature, K
V	Molar volume, cm^3/mol
V_D	Parameter in Eq. (27)

Greek letters

η	Viscosity, cP
φ_1	HS packing fraction of solvent
ρ	Number density, N_a/V, cm^{-3}
ε/k_B	Lennard–Jones energy parameter, K
σ	Molecular diameter, cm

Subscripts

bp	Boiling point
c	Critical property
eff	Effective hard sphere diameter (EHSD)
E	Enskog
HS	Hard sphere fluid
LJ	Lennard–Jones fluid
R	Reduced property
Real	Refers to real systems
1, 11	Solvent
2	Solute
12	Binary property

Superscripts

0	Ideal gas
*	Reduced quantity

contribution of attractive forces is considered by combining an Arrhenius exponential term. Such approaches are well grounded in theory [2,12,22,23].

The paper is organized as follows: the new tracer diffusion model is derived in Section 2; the equations adopted for comparison are presented in Section 3; the compiled D_{12} database and all data necessary for the calculations are given in Section 4; the calculated results and discussion constitute Section 5; in the final section, most important conclusions are drawn.

2. New tracer diffusivity model for real systems, $D_{12,Real}$

The theoretical path adopted in this essay to develop the new tracer diffusion coefficients model for real systems may be summarized as follows: (i) first, an accurate expression for the tracer diffusivity of the HS fluid ($D_{12,HS}$) will be adopted; (ii) then, the effective hard sphere diameter (EHSD) method will be used to take into account essentially the softness of the repulsive potential; (iii) the effect of the attractive forces, which play an important role especially at low temperatures, will be included by coupling an exponential energetic term with one parameter, α_{12}. The equation so obtained involves three parameters: α_{12} and the LJ force constants σ_{LJ} and ε_{LJ}/k_B; (iv) The final model will be than applied to real substances by computing σ_{LJ} and ε_{LJ}/k_B with generalized correlations, and fitting the remaining parameter to experimental data available in the literature. In the following, the new $D_{12,Real}$ model will be derived according to these steps.

The diffusion coefficient of an infinitely diluted gas, D^0_{12}, may be calculated by the rigorous kinetic theory of gases:

$$\rho^0_1 D^0_{12} = \frac{3}{8\sigma^2_{12}} \left(\frac{k_B T}{2\pi m_{12}}\right)^{1/2} \tag{1}$$

where scripts "0", "1" and "2" denote ideal gas, solvent and solute, respectively, ρ_1 is number density, k_B is Boltzmann constant, T is absolute temperature, m_{12} is the reduced mass of the system, and σ_{12} is the distance between the centers of the molecules at collision. The values of m_{12} and σ_{12} are calculated in terms of the individual molecular masses and diameters by:

$$\sigma_{12,LJ} = \frac{\sigma_{1,LJ} + \sigma_{2,LJ}}{2} \tag{2}$$

$$m_{12} = \frac{m_1 m_2}{m_1 + m_2} = \frac{1}{N_a} \frac{M_1 M_2}{M_1 + M_2} \tag{3}$$

Eq. (1) is not applicable to dense gases and liquids since it is based upon the Boltzmann equation for the distribution function. Enskog [1,2,24] corrected the ideal gas behaviour by taking into account excluded molecular volume effects, which are increasingly important as density raises, and by modifying the collision frequency in the fluid by the unlike pair radial distribution function at contact, $g(\sigma_{12})$. Accordingly, the Enskog equation for the tracer diffusion coefficient is:

$$\frac{\rho_1 D_{12,E}}{\rho^0_1 D^0_{12}} = \frac{1}{g(\sigma_{12})} \tag{4}$$

In this paper $g(\sigma_{12})$ is calculated by the expression of Mansoori et al. [25], due to its simplicity and accuracy. It depends on the solvent HS packing fraction of the solvent, φ_1, and solute solvent diameter ratio:

$$g(\sigma_{12}) = \frac{1}{(1-\varphi_1)^3} \left(1 - \varphi_1 + \frac{2\varphi_1}{1 + \sigma_1/\sigma_2}\right) \left(1 - \varphi_1 + \frac{\varphi_1}{1 + \sigma_1/\sigma_2}\right) \tag{5}$$

For N_1 spheres occupying a volume V, φ_1 is given by:

$$\varphi_1 = \frac{N_1 \pi \sigma^3_1}{6V} = \frac{\pi}{6} \rho_1 \sigma^3_1 = \frac{\pi}{6} \rho^*_1 , \quad \rho^*_1 \equiv \rho_1 \sigma^3_1 \tag{6}$$

where ρ^*_1 is the reduced number density of solvent.

The Enskog theory is not applicable over large density range since it does not take into account the correlated motions between core collisions responsible for backscattering and vortex flow effects. Hence, the HS tracer diffusivity is usually obtained by correcting Enskog theory with a correction factor (F_{12}) dependent upon the reduced density of the solvent, and on the size and mass ratios:

$$D_{12,HS} = D_{12,E} \times \left(\frac{D_{12,HS}}{D_{12,E}}\right) = D_{12,E} \times F_{12} \left(\rho^*_1, \frac{\sigma_2}{\sigma_1}, \frac{m_2}{m_1}\right) \tag{7}$$

The F_{12} correlation of Magalhães et al. [26] has been adopted in this essay, since it is simple, explicit and very accurate, in comparison to several well known models from literature as those by

Sung and Stell [27], Sun and Chen [28], Easteal and Woolf [29], and Eaton and Akgerman [30]. It is applicable in the range $0.4714 \le \rho_1^* \le 0.9428$, $0.25 \le \sigma_2/\sigma_1 \le 1.00$, $0.01 \le m_2/m_1 \le 4.00$:

$$F_{12} = \frac{F_{11} + \rho_1^{*1.7}\left[a\ln(\sigma_2/\sigma_1) + b\ln^2(\sigma_2/\sigma_1) + c\ln(m_2/m_1)\right]}{1 + \rho_1^{*3.0}\left[d\ln(\sigma_2/\sigma_1)\right]^2} \tag{8}$$

where coefficients a, b, c and d are linear functions of the reduced number density of solvent:

$$\begin{cases} a = -1.676382\rho_1^* + 1.638561 \\ b = -8.516830\rho_1^* + 8.631536 \\ c = -1.320347\rho_1^* + 1.351067 \\ d = -5.062546\rho_1^* + 5.409662 \end{cases} \tag{9}$$

and F_{11} is calculated according to Ruckenstein and Liu [31]:

$$F_{11} = 1 + 0.94605\rho_1^{*1.5} + 1.4022\rho_1^{*3} - 5.6898\rho_1^{*5} + 2.6626\rho_1^{*7} \tag{10}$$

The softness of the repulsive interactions should be now introduced. This may be accomplished by perturbation approaches, which usually combine HS models as an appealing and tractable first approximation, for the major excluded-volume and packing effects, with an effective diameter dependent on temperature and possibly on density, to account for the softness of the repulsive potential. Following Liu et al. [23,32] and the extensive comparison carried out by Silva et al. [12], the selected expression is only T-dependent:

$$\sigma_{i,\,\mathrm{eff}}(T_i^*) = \sigma_{i,\,\mathrm{LJ}} \times 2^{1/6}[1 + (1.3229\,T_i^*)^{1/2}]^{-1/6}, \quad i = 1,\ 2,\ 12 \tag{11}$$

Note that $i = 1$ or 2 for pure solvent and solute, and 12 for the binary system. According to Eq. (5), the calculation of $g(\sigma_{12,\mathrm{eff}})$ needs $\varphi_{1,\mathrm{eff}} = \pi/6\rho_1\sigma_{1,\mathrm{eff}}^3$, and effective diameters $\sigma_{1,\mathrm{eff}}$ and $\sigma_{2,\mathrm{eff}}$; additionally, F_{12} (Eq. (8)) also needs $\sigma_{1,\mathrm{eff}}$ and $\sigma_{2,\mathrm{eff}}$; on the contrary, Eq. (1) uses $\sigma_{12,\mathrm{eff}}$. The implied reduced temperatures are:

$$T_i^* \equiv \frac{k_B T}{\varepsilon_{i,\mathrm{LJ}}}, \quad i = 1,\ 2,\ 12 \tag{12}$$

where the binary LJ diameter and energy are evaluated by the classical Lorentz-Berthelot combining rules given by Eqs. (2) and (13), respectively.

$$\frac{\varepsilon_{12,\mathrm{LJ}}}{k_B} = \sqrt{\left(\frac{\varepsilon_{1,\mathrm{LJ}}}{k_B}\right) \times \left(\frac{\varepsilon_{2,\mathrm{LJ}}}{k_B}\right)} \tag{13}$$

The LJ force constants may be taken from Table 7 of Liu et al. [32] or, for substances not covered in that essay, calculated by the following corresponding states correlations of Silva et al. [22] (critical constants in K and bar):

$$\sigma_{\mathrm{LJ}}^3(\text{Å}^3) = 0.17791 + 11.779\left(\frac{T_c}{P_c}\right) - 0.049029\left(\frac{T_c}{P_c}\right)^2 \tag{14}$$

$$\frac{\varepsilon_{\mathrm{LJ}}}{k_B} = 0.774\,T_c \tag{15}$$

Eq. (14) may be adopted successfully for $T_c/P_c < 100$. For higher values, one may estimate LJ diameter by a relation provided by principles of corresponding states [13,33,34], $\sigma_{\mathrm{LJ}}(\text{Å}) = 0.809V_c^{1/3}$, where V_c is critical volume in $\mathrm{cm}^3/\mathrm{mol}$.

Let us now analyse the attractive forces. According to Kushick and Berne [35] and Straub [36], such forces play an important role in the transport process, especially at low temperatures. Several functions have been proposed in literature to take them into account in order to derive models for the LJ fluid (e.g. Straub [36], Speedy et al. [37]). In this work an exponential factor has been selected to embody such attractive contribution:

$$D_{12,\mathrm{LJ}} = D_{12,\mathrm{E}} \times F_{12} \times \exp\left(-\frac{\alpha_{12}}{T_{12}^*}\right) \tag{16}$$

The desired correlation for the tracer diffusion coefficient of real systems, $D_{12,\mathrm{Real}}$, can be now obtained by writing Eq. (16) explicitly as function of T and ρ_1. After carrying out all previous substitutions the final $D_{12,\mathrm{Real}}$ model arises:

$$D_{12,\mathrm{Real}} = \frac{3}{8\rho_1\sigma_{12,\mathrm{eff}}^2}\left(\frac{k_B T}{2\pi m_{12}}\right)^{1/2} \times \frac{F_{12}}{g(\sigma_{12,\mathrm{eff}})} \times \exp\left(-\frac{E_D}{R_g T}\right) \tag{17}$$

where $R_g = 8.31541 \times 10^7$ erg/mol K is the universal gas constant, and $E_D \equiv (\varepsilon_{12,\mathrm{LJ}}/k_B)\alpha_{12}/R_g$ is the unique parameter involved, which only depends on the binary system and can be fitted to experimental data. So, our model may be presented in condensed notation like $D_{12,\mathrm{Real}} = D_{12,\mathrm{Real}}(T, \rho_1; E_D)$. For clarity, in Fig. 1 the entire calculation procedure is schematically represented.

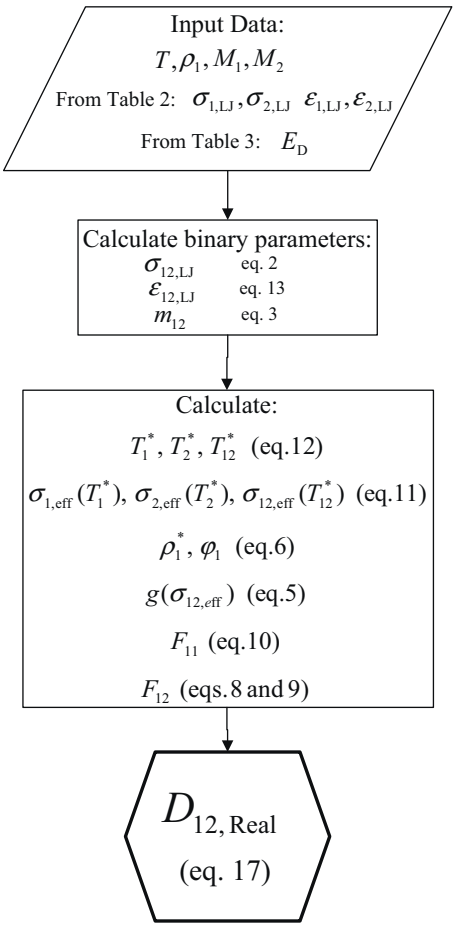

Fig. 1. Calculation procedure of new model.

3. Models adopted for comparison

In this paper five tracer diffusivity models were adopted for comparison. They are the hydrodynamic expressions of Wilke–Chang (WC), Lusis–Ratcliff (LR), and Lai–Tan (LT) with zero

parameters [3,13]; the predictive equation of Zhu et al. (Zhu) [38]; and the 2-parameter correlation of Dymond (DHB) [1,2,39]. In the following, their expressions are summarily presented.

Wilke-Chang equation [3,13,40]

$$D_{12}(\mathrm{cm^2/s}) = 7.4\times10^{-8}\frac{T\sqrt{\phi M_1}}{\eta_1 V_{\mathrm{bp},2}^{0.6}} \tag{18}$$

where ϕ is a dimensionless association factor of the solvent (for CO_2, $\phi = 1$), η_1 is the solvent viscosity (cP); M_1 is solvent molecular weight (g/mol); $V_{\mathrm{bp},2}$ is solute molar volume at its normal boiling point ($\mathrm{cm^3/mol}$).

Lusis-Ratcliff equation [3,41]

$$D_{12}(\mathrm{cm^2/s}) = \frac{8.52\times10^{-8}T}{\eta_1 V_{\mathrm{bp},1}^{1/3}}\left[1.40\left(\frac{V_{\mathrm{bp},1}}{V_{\mathrm{bp},2}}\right)^{1/3}+\left(\frac{V_{\mathrm{bp},1}}{V_{\mathrm{bp},2}}\right)\right] \tag{19}$$

Lai-Tan equation [42]

$$D_{12}\left(\mathrm{cm^2/s}\right) = 2.50\times10^{-7}\frac{T\sqrt{M_1}}{(10\times\eta_1)^{0.688}V_{\mathrm{c},2}^{1/3}} \tag{20}$$

Model of Zhu et al. [38]

$$D_{12} = \frac{3}{8\sqrt{\pi}}\sqrt{\frac{\sigma_{12,\mathrm{LJ}}^2\varepsilon_{12,\mathrm{LJ}}}{m_1}}\frac{\sqrt{T_{12}^*}}{\rho_{12}^*}\left(1-\frac{\rho_{12}^*}{1.029079T_{12}^{*0.165377}}\right)\times\left[1+\rho_{12}^{*0.126978}\left(\frac{0.596103\left(\rho_{12}^*-1\right)}{0.539292\left(\rho_{12}^*-1\right)+T_{12}^{*\left(0.400152-0.41054\rho_{12}^*\right)}}+0.68856\right)\right]\times\exp\left(-\frac{\rho_{12}^*}{2T_{12}^*}\right) \tag{21}$$

Here, T_{12}^* is calculated as before, but distinct reduced density is introduced, as $\sigma_{12,\mathrm{LJ}}$ is implied instead of $\sigma_{2,\mathrm{LJ}}$:

$$T_{12}^* = \frac{T}{\varepsilon_{12,\mathrm{LJ}}/k_\mathrm{B}},\quad \rho_{12}^* = \rho_1\sigma_{12,\mathrm{LJ}}^3 \tag{22}$$

The combining rules adopted to determine binary parameters are:

$$\varepsilon_{12,\mathrm{LJ}}/k_\mathrm{B} = \sqrt{\left(\varepsilon_{1,\mathrm{LJ}}/k_\mathrm{B}\right)\times\left(\varepsilon_{2,\mathrm{LJ}}/k_\mathrm{B}\right)}$$
$$\sigma_{12,\mathrm{LJ}} = \left(1-k_{12}^\mathrm{d}\right)\frac{\sigma_{1,\mathrm{LJ}}+\sigma_{2,\mathrm{LJ}}}{2};\quad \text{where } k_{12}^\mathrm{d} = 0.7926\frac{\sigma_{2,\mathrm{LJ}}-\sigma_{1,\mathrm{LJ}}}{\sigma_{1,\mathrm{LJ}}+\sigma_{2,\mathrm{LJ}}} \tag{23}$$

The LJ parameters for the solvent and solute are estimated by distinct expressions:

$$\varepsilon_{1,\mathrm{LJ}}/k_\mathrm{B}\,(\mathrm{K}) = \frac{T_{\mathrm{c},1}}{T_{\mathrm{c},1}^*}\left[1+0.47527332\,\rho_{\mathrm{r},1}+\left(0.06300484+0.12374707\rho_{\mathrm{r},1}\right)\,T_{\mathrm{r},1}\right] \tag{24}$$

$$\sigma_{1,\mathrm{LJ}}\,(\mathrm{cm}) = \left(\frac{\rho_{\mathrm{c},1}^*}{\rho_{\mathrm{c},1}}\right)^{1/3}\left[1-0.0368868\,\rho_{\mathrm{r},1}+\left(0.00006945+0.01089228\,\rho_{\mathrm{r},1}\right)\,T_{\mathrm{r},1}\right] \tag{25}$$

$$\frac{\varepsilon_{2,\mathrm{LJ}}}{k_\mathrm{B}} = \frac{T_{\mathrm{c},2}}{1.313}\quad\text{and}\quad \sigma_{2,\mathrm{LJ}} = \sqrt[3]{\frac{0.13\,\varepsilon_{2,\mathrm{LJ}}}{P_{\mathrm{c},2}}} \tag{26}$$

Such equations are based on the principle of corresponding states, and on the critical point computed by Johnson et al. [43] for the LJ fluid ($P_\mathrm{c}^* = 0.13,\ T_\mathrm{c}^* = 1.313,\ \rho_\mathrm{c}^* = 0.31$).

Dymond Free-Volume expression [1,2,39]

This model embodies two adjustable parameters: B is a constant characteristic of the solvent–solute pair and V_D is a constant related primarily with the solvent.

$$D_{12} = B\sqrt{T}\left(V_1 - V_\mathrm{D}\right) \tag{27}$$

4. Model validation: database and data for the calculations.

In this work the largest database of tracer diffusivities published up till now has been compiled with the purpose to validate the new $D_{12,\mathrm{Real}}$ model. It comprehends 314 systems performing 5421 points, covering gas (37 systems/422 points), liquid (104 systems/675 points) and supercritical (173 systems/4324 points) mixtures. Table 1 contains the systems studied, number of data points (NDP), number of systems (NS), reduced ranges of temperature, pressure, and solvent density for each system (reduction performed with critical constants), and data sources. As much as possible, all published data were used. However, systems with data available only in graphical form have been rejected. In Table 2 the name, molecular formula, CAS number, molecular weight, critical constants (T_c, P_c and V_c), normal boiling point (T_bp), molar volume at normal boiling point (V_bp), and LJ force constants (for the new system) are listed for all molecules involved in calculations (205 totally). All data sources are identified.

Some authors do not report the solvent densities of their data. In these cases they have been calculated by the correlations of Pitzer and Schreiber [44] for CO_2, and Hankinson-Brobst-Thomson [13,45] for other fluids. Concerning the non-reported viscosities, which are necessary for the hydrodynamic equations adopted for comparison in this work, they have been estimated by the correlations of Mehrotra [46] for liquid hydrocarbons, and Altunin and Sakhabetdinov [47] for carbon dioxide. The unknown molar volumes at normal boiling point were estimated by Tyn Calus equation [13,48]. The unknown critical constants were estimated by Joback [13,49,50], Somayajulu [51], Klincewicz [13,52], Ambrose [13,53,54], Wen-Qiang [55], and Constantinou-Gani [56] methods.

5. Results and discussion

Table 3 shows the detailed results obtained with our model – Eq. (17)/Fig. 1 – and the equations adopted for comparison: the hydrodynamic expressions of Wilke-Chang (WC) [3,13,40], Lusis-Ratcliff (LR) [3,41], and Lai-Tan (LT) [42] with zero parameters; the predictive equation of Zhu et al. (Zhu) [38]; and Dymond's correlation (DHB) [1,2,39] (2 parameters). Global results are compiled in Table 4.

Concerning the calculation procedure, the new model is explicit and straightforward. One only needs the temperature, solvent density and the diffusive energy specific for each binary system, i.e. $D_{12,\mathrm{Real}} = D_{12,\mathrm{Real}}(T, \rho_1; E_\mathrm{D})$. In this work one presents NS = 314 values of E_D in Table 3. In terms of future applications, whenever E_D is unknown, it may be firstly optimized using some data points from literature. It is worth noting this optimization is very simple to carry out, since Eq. (17) may be linearized.

Table 1
Systems studied and data sources (note: an hyphen means that data is not available.).

System		$T_{r,1}$	$P_{r,1}$	$\rho_{r,1}$	NDP	Data sources
Solvent (1)	Solute (2)					
		Supercritical systems				
2,3-dimethylbutane	benzene	1.046–1.096	1.710–5.080	1.4320–1.9083	11	[57]
	naphthalene	1.046–1.096	1.710–5.080	1.4320–1.9083	9	[57]
	phenanthrene	1.046–1.096	1.710–5.080	1.4320–1.9083	11	[57]
	toluene	1.046–1.096	2.005–5.080	1.4320–1.9083	10	[57]
carbon dioxide	1,1,1,5,5,5-hexafluoroacetylacetone	1.013–1.046	1.411–3.008	1.2102–1.8699	15	[58]
	1,1′-dimethylferrocene	1.013–1.063	1.114–5.436	0.8278–2.0767	68	[59]
	1,2-dichlorobenzene	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[60]
	1,2-diethylbenzene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[61]
	1,3,5-trimethylbenzene	0.997–1.096	1.287–4.743	1.2482–1.9104	24	[62–64]
	1,3-divinylbenzene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[65]
	1,4-diethylbenzene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[61]
	15-crown-5	1.013–1.030	1.188–4.070	0.8997–1.9430	29	[66]
	1-naphthol	1.013–1.046	1.436–2.195	1.1308–1.7453	11	[67]
	1-phenyldodecane	1.029–1.095	2.033–4.743	1.2953–1.9973	15	[68]
	1-phenylethanol	1.030–1.096	2.033–4.743	1.2955–1.9979	15	[69]
	1-phenylhexane	1.029–1.095	2.033–4.743	1.2953–1.9973	15	[68]
	1-phenyloctane	1.029–1.095	2.033–4.743	1.2953–1.9973	15	[68]
	1-propanol	1.030	1.287–2.168	1.2360–1.6971	17	[70]
	2,2,4,4-tetramethyl-3-pentanone	1.031	1.355–2.168	1.3304–1.6937	9	[71]
	2,3-dimethylaniline	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[72]
	2,3-dimethylnaphthalene	1.013	1.341–2.629	1.5133–1.8374	3	[73]
	2,4-dimethyl-3-pentanone	1.033	1.355–2.439	1.2971–1.7377	8	[71]
	2,4-dimethylphenol	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[74]
	2,6-dimethylaniline	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[72]
	2,6-dimethylnaphthalene	1.013	1.233–2.642	1.4272–1.8392	6	[73,75]
	2,7-dimethylnaphthalene	1.013	1.450–2.710	1.5707–1.8482	6	[73,75]
	2-bromoanisole	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[65]
	2-butanone	1.013–1.079	1.129–4.679	1.2427–2.0287	38	[76]
	2-ethyltoluene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[77]
	2-fluoroanisole	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[65]
	2-heptanone	1.034	1.423–2.439	1.3637–1.7339	11	[71]
	2-methylanisole	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[72]
	2-naphthol	1.013–1.079	1.341–2.060	0.7020–1.7176	16	[67]
	2-nitroanisole	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[60]
	2-nonanone	1.034	1.355–2.033	1.2820–1.6464	10	[71]
	2-pentanone	1.013–1.034	1.203–3.963	1.1841–1.9341	23	[76]
	2-phenyl-1-propanol	1.030–1.096	2.033–4.743	1.2955–1.9979	15	[69]
	2-phenylethanol	1.030–1.096	2.033–4.743	1.2955–1.9979	15	[69]
	2-phenylethyl acetate	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[78]
	2-propanol	1.030	1.287–2.304	1.2360–1.7247	18	[70]
	3-ethyltoluene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[77]
	3-nitrotoluene	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[72]
	3-pentanone	1.013–1.079	1.172–4.684	1.2610–2.0286	39	[76]
	3-phenyl-1-propanol	1.030–1.096	2.033–4.743	1.2955–1.9979	15	[69]
	3-phenylpropyl acetate	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[78]
	4-ethyltoluene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[77]
	4-heptanone	1.031	1.355–2.168	1.3304–1.6937	9	[71]
	4-methylanisole	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[72]
	5-nonanone	1.034	1.355–2.439	1.2820–1.7339	12	[71]
	5-*tert*-butyl-*m*-xylene	1.013–1.309	2.033–4.743	1.2953–2.0331	31	[61]
	6-undecanone	1.034	1.355–2.439	1.2820–1.7339	13	[71]
	acetone	0.997–1.096	1.076–5.435	0.7722–2.0762	178	[62,76,79,80]
	acridine	1.013–1.079	2.337–3.734	1.5149–1.9564	6	[81]
	adamantanone	1.031	1.355–2.033	1.3304–1.6621	8	[71]
	α-linolenic acid	1.013–1.128	1.152–4.084	1.1629–1.9845	56	[82]
	allylbenzene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[65]
	aniline	1.030–1.096	2.033–4.743	1.2959–1.9104	15	[64]
	anisole	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[74]
	anthracene	1.209–1.095	4.065–47.425	0.7681–1.9949	22	[67]
	α-pinene	1.030–1.096	1.626–2.710	0.9530–1.7986	15	[83]
	arachidonic acid (AA)	1.013–1.128	1.287–4.131	1.1880–1.9890	75	[84]
	AA ethyl ester	1.013–1.112	1.141–4.058	1.0685–1.8157	48	[85]
	α-tocopherol	1.013–1.096	1.153–4.107	1.3113–1.9871	82	[82,86,87]
	β-carotene	1.013–1.096	1.236–4.111	1.3346–1.9875	90	[82,86,87]
	behenic acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	17	[88]
	benzene	0.997–1.096	1.084–4.743	0.5974–1.9973	222	[63,89–94]
	benzoic acid	0.964–1.048	0.962–4.065	1.1462–1.9424	29	[70,95,96]
	benzyl acetate	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[78]
	benzylacetone	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[97]
	biphenyl	0.964–1.063	0.962–2.317	1.1479–1.9458	24	[96]
	β-pinene	1.030–1.096	1.626–2.710	0.9530–1.7986	15	[83]
	bromobenzene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[98]
	butyric acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	16	[99,100]

Table 1 (*Continued*)

System		$T_{r,1}$	$P_{r,1}$	$\rho_{r,1}$	NDP	Data sources
Solvent (1)	Solute (2)					
	caffeine	1.013–1.079	1.088–1.943	0.9110–1.7197	21	[42]
	capric acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	16	[99,100]
	caprylic acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	16	[99,100]
	chlorobenzene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[98]
	chrysene	0.997–1.096	2.168–3.591	1.7069–1.8776	4	[62]
	citral	1.030–1.096	1.626–2.710	0.9530–1.7986	15	[101]
	cobalt(III) acetylacetonate	1.030–1.096	1.314–5.420	1.2883–2.0413	38	[102]
	copper(II) trifluoroacetylacetonate	1.013–1.046	1.466–2.243	1.2844–1.7589	12	[58]
	cycloheptanone	1.033	1.355–2.439	1.2971–1.7377	8	[103]
	cyclononanone	1.033	1.355–2.439	1.2971–1.7377	8	[103]
	cyclopentanone	1.033	1.355–2.439	1.2971–1.7377	8	[103]
	dibenzo-24-crown-8	1.013–1.030	2.034–4.743	1.6664–2.0237	28	[66]
	dibenzyl ether	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[78]
	diethyl ether	1.030–1.096	1.098–2.197	0.4182–1.7041	15	[104]
	diisopropyl ether	1.030–1.096	1.098–2.197	0.4182–1.7041	15	[104]
	diolein	1.030	1.355–3.389	1.3414–1.8777	9	[105]
	D-limonene	1.030–1.096	1.626–2.710	0.9530–1.7986	15	[101]
	docosahexaenoic acid (DHA)	1.013–1.128	1.256–4.083	1.2190–1.9849	63	[106]
	DHA ethyl ester	1.013–1.112	1.141–4.058	1.0685–1.8157	65	[85,88]
	DHA methyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	17	[88]
	eicosapentaenoic acid (EPA)	1.013–1.128	1.176–4.085	1.1571–1.9514	55	[106]
	EPA ethyl ester	1.013–1.112	1.141–4.058	1.0685–1.8157	48	[85]
	EPA methyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	17	[88]
	ethanol	1.030	1.287–3.388	1.2360–1.8776	24	[70]
	ethyl acetate	1.013–1.079	1.024–1.938	0.4545–1.7197	15	[42]
	ethyl benzoate	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[97]
	ethylbenzene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[90]
	eugenol	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[97]
	ferrocene	1.013–1.063	1.087–5.466	0.6002–2.0771	98	[59]
	fluorobenzene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[98]
	γ-linolenic acid	1.013–1.128	1.176–4.133	0.9758–1.9482	142	[107]
	γ-linolenic acid ethyl ester	1.030–1.128	1.138–2.169	0.7165–1.6974	41	[107]
	γ-linolenic acid methyl ester	1.030–1.128	1.099–4.553	0.6222–1.9821	52	[107,108]
	hexachlorobenzene	1.013–1.079	1.310–3.352	0.8698–1.9223	14	[109]
	iodobenzene	1.029–1.095	2.033–4.743	1.2959–1.9104	15	[98]
	i-propylbenzene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[90]
	L-carvone	1.013–1.112	2.033–4.065	1.3894–1.9838	23	[110]
	Linalool	1.030–1.096	1.626–2.710	0.9530–1.7986	15	[89]
	linoleic acid	1.013–1.128	1.152–4.106	1.1880–1.9870	71	[84]
	linoleic acid methyl ester	1.013–1.079	1.897–4.553	1.5767–1.9821	21	[108,111]
	L-menthone	1.013–1.112	2.033–4.065	1.3894–1.9838	23	[110]
	methanol	1.030	1.287–2.846	1.2360–1.8121	10	[70]
	monoolein	1.030	1.356–3.388	1.3430–1.8776	11	[105]
	myristic acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	16	[99,100]
	myristoleic acid	1.030–1.128	1.247–4.065	0.9770–1.8776	42	[112]
	myristoleic acid methyl ester	1.030–1.128	1.084–1.897	0.4807–1.2360	79	[112]
	N-(4-methoxybenzy-lidene)-4-*n*-butylaniline	1.031	1.626–2.168	1.5271–1.6937	5	
	naphthalene	0.948–1.096	0.911–13.550	0.6480–2.3739	83	[62,73,113,114]
	n-butylbenzene	1.029–1.095	2.033–4.743	1.2953–1.9973	15	[68]
	n-decane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-dodecane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-heptane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-hexane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	nitrobenzene	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[74]
	n-nonane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-octane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-pentane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-pentylbenzene	1.013–1.309	2.033–4.743	1.2955–2.0343	31	[68]
	n-propylbenzene	1.013–1.096	1.152–4.743	0.7638–1.9973	34	[63,90]
	n-tetradecane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	n-undecane	0.984–1.013	1.220–1.423	1.5592–1.7450	5	[115]
	oleic acid	1.030	1.282–4.079	1.2246–1.9436	19	[105]
	oleic acid ethyl ester	1.030	1.165–1.491	0.8052–1.4594	5	[105]
	oleic acid methyl ester	1.030	1.084–1.491	0.5939–1.4594	19	[105]
	palladium(II) acetylacetonate	1.013–1.128	1.152–5.420	1.2016–2.0757	125	[102]
	palmitic acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	17	[116]
	p-dichlorobenzene	0.980–1.046	1.252–2.317	1.1479–1.8669	13	[96]
	phenanthrene	0.997–1.096	1.308–3.591	1.0821–1.9242	19	[62,109]
	phenol	1.013–1.079	1.089–4.103	0.7574–1.9868	109	[42,70,80,86,87]
	phenylacetic acid	1.013–1.046	1.310–2.852	1.2802–1.8136	16	[117]
	phenylacetylene	1.030–1.096	2.033–4.743	1.2953–1.9973	15	[61]

Table 1 (*Continued*)

System		$T_{r,1}$	$P_{r,1}$	$\rho_{r,1}$	NDP	Data sources
Solvent (1)	Solute (2)					
	phenylmethanol	1.030–1.096	2.033–4.743	1.2955–1.9979	15	[69]
	pyrene	1.209–1.095	14.499–47.425	0.8321–1.9885	18	[67]
	squalene	1.034	1.762–2.439	1.5621–1.7339	5	[71]
	stearic acid ethyl ester	1.013–1.046	1.310–2.852	1.2802–1.8136	17	[88]
	styrene	1.030–1.096	2.033–4.743	1.2959–1.9104	15	[64]
	tert-butylbenzene	1.029–1.095	2.033–4.743	1.2955–1.9971	15	[60]
	tetrahydrofuran	1.030–1.096	1.098–2.197	0.4182–1.7041	15	[104]
	thenoyltrifluoroacetone	1.013–1.046	1.430–3.037	1.2102–1.8870	15	[58]
	toluene	1.007–1.096	1.089–4.743	0.9687–1.9973	35	[42,90,94]
	triarachidonin	1.030	1.348–4.098	1.3330–1.9452	27	[118]
	trierucin	1.013–1.063	1.119–4.073	1.2041–1.9840	101	[105]
	trifluoroacetylacetone	1.013–1.046	1.449–2.924	1.2375–1.8731	15	[58]
	trinervonin	1.013–1.063	1.220–4.072	1.2680–1.9841	38	[105]
	triolein	1.030	1.237–1.900	1.1011–1.6305	10	[105]
	ubiquinone CoQ10	1.013–1.096	1.153–4.095	1.3113–1.9844	80	[87,119]
	vanillin	1.013–1.046	1.396–2.852	1.2802–1.8136	15	[117]
	vitamin K_1	1.030	1.355–4.065	1.3418–1.9425	16	[66]
	vitamin K_3	1.030	1.214–4.068	1.0177–1.9432	20	[87,111]
chlorotrifluoromethane	acetone	1.037	1.150-2.093	0.6873–1.6510	10	[120]
	p-xylene	1.053	1.220–2.819	0.6908–1.7270	8	[120]
ethane	1-octene	0.970–1.055	1.449–2.295	1.5210–1.9683	6	[121]
	1-tetradecene	0.960–1.055	1.414–2.295	1.5190–1.9925	9	[121]
sulfur hexafluoride	1,3,5-trimethylbenzene	1.029	1.117-3.816	0.6806–1.9056	10	[120]
	benzene	1.029	0.931-3.816	0.4083–1.9056	9	[120]
	benzoic acid	1.030–1.061	1.729–3.191	1.2485–1.9065	6	[116]
	carbon tetrachloride	1.029	1.117-3.816	0.6806–1.9056	6	[120]
	naphthalene	0.998–1.030	1.729–3.191	1.5089–2.0278	5	[116]
	p-xylene	0.889–1.061	0.798–3.989	0.4083–2.2459	52	[120]
	toluene	1.029	0.931-3.816	0.4083–1.9056	11	[120]
		Liquid systems				
2,2,4-trimethylpentane	1,3,5-trimethylbenzene	0.557–0.612	-	2.7566–2.8675	4	[122]
	benzene	0.557–0.612	-	2.7566–2.8675	4	[122]
	ethylbenzene	0.557–0.612	-	2.7566–2.8675	4	[122]
	o-xylene	0.557–0.612	-	2.7566–2.8675	4	[122]
	p-xylene	0.557–0.612	-	2.7566–2.8675	4	[122]
	toluene	0.557–0.612	-	2.7566–2.8675	4	[122]
cyclohexane	1,1′-dimethylferrocene	0.566–0.584	0.047–4.673	2.7456–2.7799	5	[123]
	1,3,5-trimethylbenzene	0.539–0.945	3.931; sat.p.a	1.7566–2.8618	12	[28,124]
	argon	0.566–0.751	-	2.3861–2.7813	6	[125]
	benzene	0.539–0.945	3.931; sat.p.	1.7566–2.8618	12	[28,124]
	carbon tetrachloride	0.566–0.751	-	2.3861–2.7813	6	[125]
	ethane	0.507–0.656	-	2.5947–2.9057	5	[126]
	ethylene	0.507–0.656	-	2.5947–2.9057	5	[126]
	ethylferrocene	0.566–0.584	0.042–4.673	2.7456–2.7799	6	[123]
	ferrocene	0.566–0.584	0.047–4.673	2.7456–2.7799	5	[123]
	krypton	0.566–0.751	-	2.3861–2.7813	6	[125]
	methane	0.566–0.751	-	2.3861–2.7813	6	[125]
	naphthalene	0.539–0.945	3.931; sat.p.	1.7566–2.8618	12	[28,124]
	phenanthrene	0.539–0.945	sat.p.	1.7566–2.8325	8	[28]
	p-xylene	0.539–0.945	sat.p.	1.7566–2.8325	8	[28]
	tetrabutyltin	0.539–0.751	-	2.3861–2.8325	7	[125]
	tetraethyltin	0.539–0.751	-	2.3861–2.8325	7	[125]
	tetramethyltin	0.539–0.751	-	2.3861–2.8325	7	[125]
	tetrapropyltin	0.539–0.751	-	2.3861–2.8325	6	[125]
	toluene	0.539–0.945	3.931; sat.p.	1.7566–2.8618	12	[28,124]
	xenon	0.539–0.751	-	2.3861–2.8325	6	[125]
n-decane	12-crown-4	0.483–0.604	-	2.8291–3.0824	4	[127]
	15-crown-5	0.483–0.604	-	2.8291–3.0824	4	[127]
	18-crown-6	0.483–0.604	-	2.8291–3.0824	4	[127]
	argon	0.482–0.701	-	2.6077–3.0831	3	[128]
	carbon tetrachloride	0.482–0.604	-	2.8298–3.0831	3	[128]
	dicyclohexano-18-crown-6	0.483–0.604	-	2.8291–3.0824	4	[127]
	dicyclohexano-24-crown-8	0.483–0.604	-	2.8291–3.0824	4	[127]
	krypton	0.482–0.701	-	2.6077–3.0831	3	[128]
	methane	0.482–0.701	-	2.6077–3.0831	3	[128]
	s-trioxane	0.483–0.604	-	2.8291–3.0824	4	[127]
	tetrabutyltin	0.482–0.701	-	2.6077–3.0831	4	[128]
	tetraethyltin	0.482–0.701	-	2.6077–3.0831	3	[128]
	tetramethyltin	0.482–0.701	-	2.6077–3.0831	4	[128]
	tetrapropyltin	0.482–0.701	-	2.6077–3.0831	4	[128]
	xenon	0.482–0.701	-	2.6077–3.0831	4	[128]
n-dodecane	1,3,5-trimethylbenzene	0.461–0.506	8.791	3.0682–3.1519	4	[124]
	acetone	0.461–0.521	8.791	3.0389–3.1519	5	[124]
	benzene	0.461–0.506	8.791	3.0682–3.1519	4	[124]
	carbon dioxide	0.462–0.862	0.765–1.898	2.1292–3.1028	9	[129]

Table 1 (*Continued*)

System		$T_{r,1}$	$P_{r,1}$	$\rho_{r,1}$	NDP	Data sources
Solvent (1)	Solute (2)					
	carbon monoxide	0.462–0.862	0.765–1.898	2.1292–3.1028	9	[129]
	hydrogen	0.462–0.862	0.765–1.898	2.1292–3.1028	9	[129]
	linoleic acid methyl ester	0.461–0.506	8.791	3.0682–3.1519	4	[124]
	m-xylene	0.461–0.506	8.791	3.0682–3.1519	4	[124]
	naphthalene	0.461–0.521	8.791	3.0389–3.1519	5	[124]
	n-decane	0.462–0.860	0.776–0.796	2.1896–3.1067	5	[130]
	n-hexadecane	0.462–0.860	0.776–0.796	2.1896–3.1067	5	[130]
	n-octane	0.462–0.860	0.776–1.890	2.1896–3.1067	9	[130]
	n-tetradecane	0.462–0.860	0.776–0.796	2.1896–3.1067	5	[130]
	toluene	0.461–0.506	8.791	3.0682–3.1519	4	[124]
n-eicosane	carbon dioxide	0.488–0.696	1.226	2.6453–3.1064	5	[131]
	carbon monoxide	0.488–0.696	1.226	2.6453–3.1064	5	[131]
	hydrogen	0.488–0.696	1.226	2.6453–3.1064	5	[131]
	n-dodecane	0.489–0.696	1.226	2.6449–3.1064	5	[131]
	n-hexadecane	0.489–0.696	1.226	2.6449–3.1064	5	[131]
	n-octane	0.489–0.696	1.226	2.6449–3.1064	5	[131]
n-heptane	*n*-decane	0.553–0.883	0.037–1.268	2.2353–2.9290	5	[130]
	n-dodecane	0.553–0.883	0.037–1.296	2.2353–2.9437	5	[130]
	n-hexadecane	0.553–0.883	0.037–1.296	2.1638–2.9437	8	[130]
	n-octane	0.553–0.883	0.037–1.268	2.2353–2.9290	4	[130]
	n-tetradecane	0.553–0.883	0.037–1.296	2.2353–2.9437	5	[130]
n-hexadecane	carbon dioxide	0.448–0.781	0.991–2.454	2.3098–3.0928	10	[129]
	carbon monoxide	0.448–0.781	0.991–2.454	2.3098–3.0928	10	[129]
	hydrogen	0.448–0.781	0.991–2.454	2.3098–3.0928	10	[129]
	n-decane	0.448–0.781	1.004–1.021	2.3606–3.0917	5	[132]
	n-dodecane	0.448–0.781	1.004–1.021	2.3606–3.0917	5	[132]
	n-octane	0.448–0.781	1.004–2.486	2.3606–3.0950	10	[132]
	n-tetradecane	0.448–0.781	1.004–1.021	2.3606–3.0917	5	[132]
n-hexane	1,1′-dimethylferrocene	0.617	0.056–6.319	2.7590–2.7591	4	[123]
	1,3,5-trimethylbenzene	0.597–1.070	b	1.3481–2.8637	20	[124,133]
	acetone	0.597–0.657	5.316	2.7521–2.8637	5	[124]
	acetonitrile	0.588	0.034–128.11	2.8122–3.4674	7	[134]
	benzene	0.588–1.070	c	1.3481–3.4493	36	[124,126,133,134]
	carbon disulphide	0.588	0.034–127.575	2.8122–3.4665	10	[134]
	ethylferrocene	0.617	0.053–6.316	2.7590–2.7591	4	[123]
	ferrocene	0.617	0.053–6.316	2.7590–2.7591	4	[123]
	indole	0.617	5.316–8.306	2.7907–2.8637	4	[111,124]
	m-xylene	0.597–0.657	5.316	2.7521–2.8637	5	[124]
	naphthalene	0.597–1.070	b	1.3481–2.8637	20	[124,133,134]
	phenanthrene	0.657–1.070	sat.p.; $P_{r,1} > 1$	1.3481–2.6705	15	[133]
	p-xylene	0.617–1.070	b	1.3481–2.8637	17	[124,133]
	toluene	0.588–1.070	d	1.3481–3.4592	28	[124,133]
n-octane	1,3,5-trimethylbenzene	0.533–0.586	-	2.8882–2.9974	4	[122]
	argon	0.524–0.709	-	2.5858–3.0098	4	[128]
	benzene	0.533–0.586	-	2.8882–2.9974	4	[122]
	carbon tetrachloride	0.524–0.656	-	2.7361–3.0098	4	[128]
	ethyl benzene	0.533–0.586	-	2.8882–2.9974	4	[122]
	krypton	0.524–0.709	-	2.5858–3.0098	4	[128]
	methane	0.524–0.709	-	2.5858–3.0098	4	[128]
	o-xylene	0.533–0.586	-	2.8882–2.9974	4	[122]
	p-xylene	0.533–0.586	-	2.8882–2.9974	4	[122]
	tetrabutyltin	0.524–0.761	-	2.4799–3.0159	4	[128]
	tetraethyltin	0.524–0.761	-	2.4799–3.0159	5	[128]
	tetramethyltin	0.524–0.761	-	2.4799–3.0159	4	[128]
	tetrapropyltin	0.524–0.761	-	2.4799–3.0159	4	[128]
	toluene	0.533–0.586	-	2.8882–2.9974	4	[122]
	xenon	0.524–0.709	-	2.5858–3.0098	4	[128]
propane	1-octene	0.802–0.913	1.308–2.198	2.0441–2.3664	8	[121]
	1-tetradecene	0.791–0.912	2.092–2.165	2.1270–2.3848	8	[121]
			Gas systems			
argon	ethane	2.035–4.464	0.021	0.0014–0.0030	9	[135]
	hydrogen	0.782–1.963	0.021	0.0031–0.0077	5	[136]
	i-butane	2.026–4.464	0.021	0.0014–0.0030	8	[135]
	methane	2.043–4.464	0.021	0.0014–0.0030	9	[135]
	n-butane	2.032–4.464	0.021	0.0014–0.0030	8	[135]
	neon	0.782–9.041	0.021	0.0007–0.0077	25	[136–138]
	propane	2.027–4.503	0.021	0.0013–0.0030	9	[135]
carbon dioxide	ethylene	0.981–1.145	0.146–2.752	0.0365–1.6855	48	[139]
	hydrogen	1.037–1.131	0.014	0.0033–0.0036	7	[140]
carbon monoxide	helium	2.372–2.588	0.029	0.0033–0.0036	7	[140]
	hydrogen	2.372–2.588	0.029	0.0033–0.0036	7	[140]
deuterium	hydrogen	2.995–7.682	0.061	0.0025–0.0064	5	[136]
ethane	nitrogen	1.022–2.198	0.021	0.0027–0.0058	14	[140,141]
ethylene	carbon dioxide	1.056–1.233	0.217–3.724	0.0514–1.5935	49	[139]
	nitrogen	1.143–1.593	0.020	0.0035–0.0049	7	[140]

Table 1 (*Continued*)

System		$T_{r,1}$	$P_{r,1}$	$\rho_{r,1}$	NDP	Data sources
Solvent (1)	Solute (2)					
helium	hydrogen	22.736–176.686	0.446	0.0008–0.0059	17	[136,142]
krypton	argon	1.619–5.708	0.018	0.0009–0.0033	6	[143]
	helium	1.710–5.703	0.018	0.0009–0.0031	6	[143]
	neon	1.304–5.838	0.018	0.0009–0.0041	17	[138,143]
	xenon	1.713–5.313	0.018	0.0010–0.0031	8	[143]
methane	carbon dioxide	1.502–1.932	0.022	0.0033–0.0042	10	[144]
	tetrachloroethene	1.487–1.802	0.022	0.0035–0.0043	5	[145]
neon	deuterium	2.590–6.644	0.037	0.0017–0.0044	5	[136]
	helium	1.725–8.874	0.037	0.0013–0.0066	24	[136–138]
	hydrogen	2.590–6.644	0.037	0.0017–0.0044	5	[136]
	xenon	6.149–8.874	0.037	0.0013–0.0019	6	[138]
nitrogen	helium	2.363–3.947	0.030	0.0022–0.0037	8	[146]
	hydrogen	2.402–3.591	0.030	0.0024–0.0036	29	[147]
	methane	2.486–5.319	0.030	0.0016–0.0035	7	[141]
	n-butane	2.484–5.319	0.030	0.0016–0.0035	5	[141]
	propane	2.508–5.319	0.030	0.0016–0.0035	6	[141]
oxygen	helium	1.929–3.222	0.020	0.0018–0.0030	8	[146]
	hydrogen	1.961–2.931	0.020	0.0020–0.0030	13	[147]
sulfur hexafluoride	cyclohexane	0.888–1.077	0.027	0.0071–0.0086	5	[148]
	methylcyclohexane	0.888–1.077	0.027	0.0071–0.0086	5	[148]
tetrafluoromethane	1,1,1-trichloroethane	1.244–1.508	0.027	0.0050–0.0060	5	[145]
	tetrachloroethene	1.244–1.508	0.027	0.0050–0.0060	5	[145]

[a] sat. p: saturation pressure. [b] $P_{r,1}$ = 0.498 and 0.532, at saturation pressure and other points at $P_{r,1} > 1$. [c] $P_{r,1}$ from 0.034 to 122.69 and at saturation pressure. [d] $P_{r,1}$ from 0.034 to 124.58 and at saturation pressure.

From Table 3 it is possible to emphasize its reliability and accuracy, as it provides systematically low average absolute relative deviations (*AARDs*) for almost all solvent-solute pairs, whether in gas, liquid or supercritical state. For the 314 systems and 5421 points of the collected database, the grand *AARD* found is only 4.37% (see Table 4), which makes it a very confident 1-parameter correlation. It should be detached the notable performance achieved for systems whose LJ parameters were calculated using critical constants also estimated: e.g. systems containing 1,1′-dimethylferrocene, cobalt(III) acetylacetonate, copper(II) trifluoroacetylacetonate, dibenzo-24-crown-8, ferrocene,γ-linolenic acid ethyl ester, *N*-(4-methoxybenzylidene)-4-*n*-butylaniline, palladium(II) acetylacetonate, squalene, tetrabutyltin, thenoyltrifluoroacetone, triarachidonin, triolein, ubiquinone CoQ10, vitamin K_1,

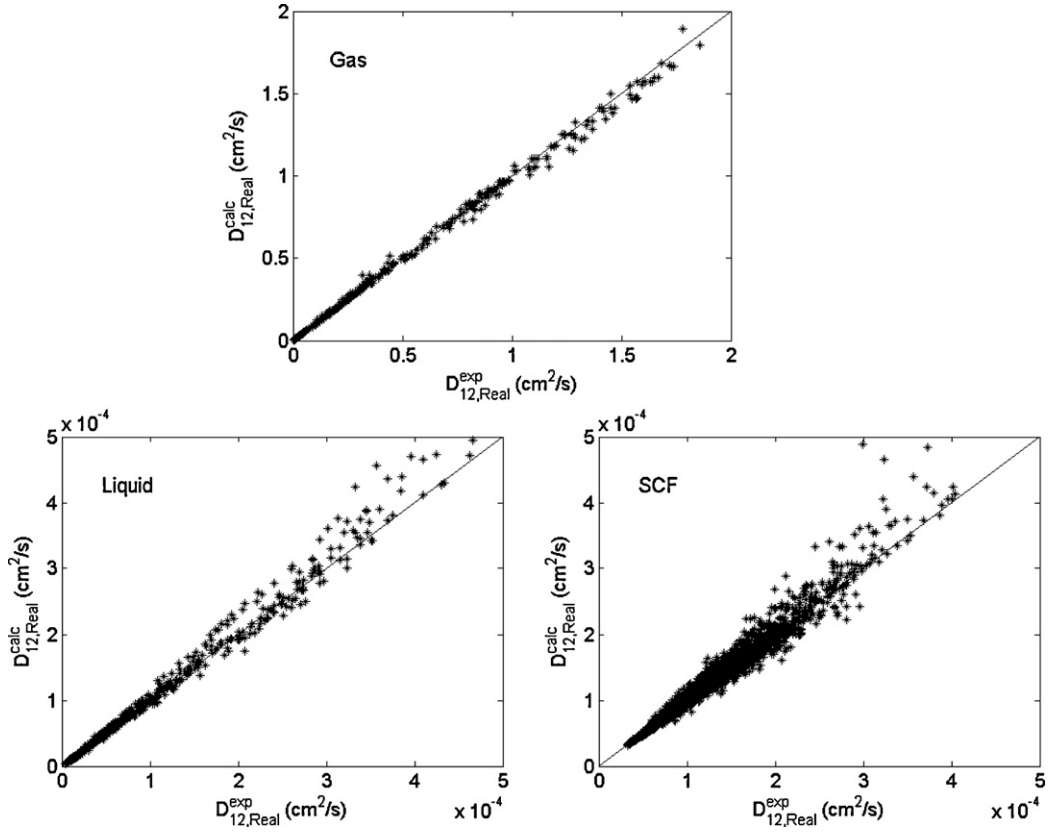

Fig. 2. Comparison between calculated and experimental tracer diffusivities for gas, liquid and supercritical systems.

Table 2
Data for pure substances.

Substance	Formula	CAS number	M (g/mol)	T_c (K)	P_c (bar)	V_c (cm^3/mol)	T_{bp} (K)	V_{bp}^m (cm^3/mol)	σ_{LJ} (Å)	ε_{LJ}/k_B (K)
1,1,1,5,5,5-hexafluoroacetylacetone	$C_5H_2F_6O_2$	1552-22-1	208.06	569.07[a]	27.17[a]	406.05[a]	410.70[j]	154.40	6.08561[p]	440.46[p]
1,1,1-trichloroethane	$C_2H_3Cl_3$	71-55-6	133.41	545.00[b]	43.00[b]	281.00[d]	347.20[b]	104.98	5.21212[p]	421.83[p]
1,1′-dimethylferrocene	$C_{12}H_{14}Fe$	1291-47-0	214.09	514.45[c]	27.41[c]	400.64[c]	353.55[k]	152.24	5.88660[p]	398.18[p]
1,2-dichlorobenzene	$C_6H_4Cl_2$	95-50-1	147.00	729.00[b]	41.00[b]	360.00[b]	452.00[b]	136.10	5.79009[p]	564.25[p]
1,2-diethylbenzene	$C_{10}H_{14}$	135-01-3	134.22	668.00[d]	28.80[d]	502.00[d]	456.61[d]	192.83	6.27438[p]	517.03[p]
1,3,5-trimethylbenzene	C_9H_{12}	108-67-8	120.20	637.30[b]	31.30[b]	433.00[d]	437.90[b]	165.15	6.03392[p]	493.27[p]
1,3-divinylbenzene	$C_{10}H_{10}$	108-57-6	130.19	692.00[d]	31.20[d]	440.00[d]	472.65[d]	167.95	6.19117[p]	535.61[p]
1,4-diethylbenzene	$C_{10}H_{14}$	105-05-5	134.22	657.96[d]	28.03[d]	497.00[d]	456.94[d]	190.82	6.29672[p]	509.26[p]
12-crown-4	$C_8H_{16}O_4$	294-93-9	176.21	780.66[e]	33.59[e]	444.75[e]	540.08[j]	169.85	6.27811[p]	604.23[p]
15-crown-5	$C_{10}H_{20}O_5$	33100-27-5	220.27	876.80[e]	28.72[e]	548.75[e]	625.60[j]	211.69	6.79750[p]	678.64[p]
18-crown-6	$C_{12}H_{24}O_6$	17455-13-9	264.32	970.51[e]	24.95[e]	652.75[e]	711.12[j]	253.92	7.26959[p]	751.17[p]
1-naphthol	$C_{10}H_8O$	90-15-3	144.17	802.00[d]	47.37[d]	375.50[d]	561.15[d]	142.24	5.70365[p]	620.75[p]
1-octene	C_8H_{16}	111-66-0	112.22	566.70[b]	26.20[b]	464.00[b]	394.40[b]	177.56	6.14478[p]	438.63[p]
1-phenyldodecane	$C_{18}H_{30}$	123-01-3	246.44	774.26[d]	15.79[d]	1000.00[d]	600.76[d]	397.05	7.71873[p]	599.28[p]
1-phenylethanol	$C_8H_{10}O$	98-85-1	122.17	675.30[f]	40.60[f]	392.15[f]	478.16[l]	148.86	5.67259[p]	522.68[p]
1-phenylhexane	$C_{12}H_{18}$	1077-16-3	162.28	698.00[d]	23.80[d]	618.00[d]	499.26[d]	239.77	6.71996[p]	540.25[p]
1-phenyloctane	$C_{14}H_{22}$	2189-60-8	190.33	729.00[d]	20.20[d]	703.00[d]	537.55[d]	274.44	7.12309[p]	564.25[p]
1-propanol	C_3H_8O	71-23-8	60.10	536.80[b]	51.70[b]	219.00[b]	370.30[b]	80.84	4.49190[q]	2120.83[q]
1-tetradecene	$C_{14}H_{28}$	1120-36-1	196.38	689.00[a]	15.60[b]	817.00[d]	524.30[b]	321.26	7.51715[p]	533.29[p]
2,2,4,4-tetramethyl-3-pentanone	$C_9H_{18}O$	815-24-7	142.24	627.18[c]	30.29[c]	407.72[c]	425.35[k]	155.06	6.06460[p]	485.44[p]
2,2,4-trimethylpentane	C_8H_{18}	540-84-1	114.23	544.00[b]	25.70[b]	468.00[b]	372.40[b]	179.17	6.10500[p]	421.06[p]
2,3-dimethylaniline	$C_8H_{11}N$	87-59-2	121.18	717.00[f]	36.30[f]	400.38[f]	494.66[l]	152.14	5.97871[p]	554.96[p]
2,3-dimethylbutane	C_6H_{14}	79-29-8	86.18	500.00[b]	31.30[b]	358.00[b]	331.10[b]	135.31	5.60227[p]	387.00[p]
2,3-dimethylnaphthalene	$C_{12}H_{12}$	581-40-8	156.23	777.78[d]	30.06[d]	521.50[d]	541.16[d]	200.69	6.48023[p]	602.00[p]
2,4-dimethyl-3-pentanone	$C_7H_{14}O$	565-80-0	114.19	597.13[c]	35.22[c]	324.85[c]	400.85[k]	122.20	5.70611[p]	462.18[p]
2,4-dimethylphenol	$C_8H_{10}O$	105-67-9	122.17	707.60[b]	44.00[d]	390.00[d]	484.10[b]	148.01	5.61388[p]	547.68[p]
2,6-dimethylaniline	$C_8H_{11}N$	87-62-7	121.18	722.00[g]	42.00[g]	400.38[f]	491.05[g]	152.14	5.73044[p]	558.83[p]
2,6-dimethylnaphthalene	$C_{12}H_{12}$	581-42-0	156.23	777.00[d]	31.70[d]	520.00[d]	535.15[d]	200.09	6.37790[p]	601.40[p]
2,7-dimethylnaphthalene	$C_{12}H_{12}$	582-16-1	156.23	778.00[d]	31.70[d]	520.00[d]	536.15[d]	200.09	6.38032[p]	602.17[p]
2-bromoanisole	C_7H_7BrO	578-57-4	187.04	737.58[f]	40.04[f]	378.05[f]	489.16[l]	143.26	5.85312[p]	570.89[p]
2-butanone	C_4H_8O	78-93-3	72.11	536.80[b]	42.10[b]	267.00[b]	352.70[b]	99.50	5.22195[p]	415.48[p]
2-ethyltoluene	C_9H_{12}	611-14-3	120.20	651.00[b]	30.40[b]	460.00[b]	438.30[b]	175.96	6.12635[p]	503.87[p]
2-fluoroanisole	C_7H_7FO	321-28-8	126.13	644.81[f]	38.11[f]	328.87[f]	427.66[l]	123.79	5.70253[p]	499.08[p]
2-heptanone	$C_7H_{14}O$	110-43-0	114.19	611.50[b]	34.40[b]	421.00[d]	424.20[b]	160.36	5.78966[p]	473.30[p]
2-methylanisole	$C_8H_{10}O$	578-58-5	122.17	648.79[f]	35.60[f]	371.70[f]	444.16[l]	140.74	5.83396[p]	502.16[p]
2-naphthol	$C_{10}H_8O$	135-19-3	144.17	811.40[i]	47.40[i]	375.50[i]	558.65[k]	142.24	5.72302[p]	628.02[p]
2-nitroanisole	$C_7H_7NO_3$	91-23-6	153.14	782.00[d]	37.60[d]	422.00[d]	546.15[d]	160.76	6.07271[p]	605.27[p]
2-nonanone	$C_9H_{18}O$	821-55-6	142.24	644.29[d]	24.53[d]	545.50[d]	346.95[g]	210.38	6.50874[p]	498.68[p]
2-pentanone	$C_5H_{10}O$	107-87-9	86.13	561.10[b]	36.90[b]	301.00[b]	375.40[b]	112.82	5.51733[p]	434.29[p]
2-phenyl-1-propanol	$C_9H_{12}O$	1123-85-9	136.20	662.02[f]	36.90[f]	443.23[f]	476.16[l]	169.24	5.80605[p]	512.40[p]
2-phenylethanol	$C_8H_{10}O$	60-12-8	122.17	684.00[d]	39.20[d]	387.00[d]	492.05[d]	146.81	5.75677[p]	529.42[p]
2-phenylethyl acetate	$C_{10}H_{12}O_2$	103-45-5	164.10	712.23[f]	30.12[f]	524.15[f]	505.16[l]	201.76	6.31046[p]	551.27[p]
2-propanol	C_3H_8O	67-63-0	60.10	508.30[b]	47.60[b]	220.00[b]	355.40[b]	81.23	4.93749[p]	393.42[p]
3-ethyltoluene	C_9H_{12}	620-14-4	120.20	637.00[b]	28.40[b]	490.00[b]	434.50[b]	188.01	6.21196[p]	493.04[p]
3-nitrotoluene	$C_7H_7NO_2$	99-08-1	137.14	734.00[d]	38.00[d]	441.00[d]	505.00[d]	168.35	5.93831[p]	568.12[p]
3-pentanone	$C_5H_{10}O$	96-22-0	86.13	561.00[b]	37.30[b]	336.00[b]	375.10[b]	126.60	5.49858[p]	434.21[p]
3-phenyl-1-propanol	$C_9H_{12}O$	122-97-4	136.20	702.30[f]	36.40[f]	455.45[f]	508.16[l]	174.14	5.93627[p]	543.58[p]
3-phenylpropyl acetate	$C_{11}H_{14}O_2$	122-72-5	178.30	718.70[f]	27.23[f]	580.37[f]	518.16[l]	224.50	6.51801[p]	556.27[p]
4-ethyltoluene	C_9H_{12}	622-96-8	120.20	640.00[b]	29.40[b]	470.00[b]	435.20[b]	179.97	6.15660[p]	495.36[p]
4-heptanone	$C_7H_{14}O$	123-19-3	114.19	595.31[d]	29.96[d]	433.50[d]	416.67[g]	165.35	5.98953[p]	460.77[p]
4-methylanisole	$C_8H_{10}O$	104-93-8	122.17	655.36[f]	35.60[f]	371.70[f]	448.66[l]	140.74	5.85195[p]	507.25[p]
5-nonanone	$C_9H_{18}O$	502-56-7	142.24	640.00[g]	23.20[h]	560.00[h]	461.60[g]	216.24	6.60236[p]	495.36[p]
5-*tert*-butyl-*m*-xylene	$C_{12}H_{18}$	98-19-1	162.28	684.85[f]	23.90[f]	591.75[f]	480.16[l]	229.11	6.67527[p]	530.07[p]
6-undecanone	$C_{11}H_{22}O$	927-49-1	170.30	678.50[h]	20.52[h]	692.00[h]	500.55[h]	269.95	6.95240[p]	525.16[p]
acetone	C_3H_6O	666-52-4	58.08	508.10[b]	47.00[b]	209.00[b]	329.20[b]	76.98	4.67012[q]	332.97[q]

Table 2 (*Continued*)

Substance	Formula	CAS number	M (g/mol)	T_c (K)	P_c (bar)	V_c (cm^3/mol)	T_{bp} (K)	V_{bp}^m (cm^3/mol)	σ_{LJ} (Å)	ε_{LJ}/k_B (K)
acetonitrile	C_2H_3N	75-05-8	41.05	545.50[b]	48.30[b]	173.00[b]	354.80[b]	63.14	4.02424[q]	652.53[q]
acridine	$C_{13}H_9N$	260-94-6	179.22	905.00[h]	36.40[h]	543.00[h]	619.15[h]	209.37	6.40475[p]	700.47[p]
adamantanone	$C_{10}H_{14}O$	700-58-3	150.22	759.15[c]	31.55[c]	368.22[c]	519.85[k]	139.36	6.34311[p]	587.58[p]
α-linolenic acid	$C_{18}H_{30}O_2$	463-40-1	278.44	780.00[h]	14.40[h]	1070.00[h]	632.00[h]	426.23	7.90702[p]	603.72[p]
allylbenzene	C_9H_{10}	300-57-2	118.18	639.86[f]	33.50[f]	419.80[f]	429.16[l]	159.88	5.91809[p]	495.25[p]
aniline	C_6H_7N	62-53-3	93.13	699.00[b]	53.10[b]	274.00[b]	457.60[b]	102.24	5.27450[p]	541.03[p]
anisole	C_7H_8O	100-66-3	108.14	641.65[d]	41.75[d]	337.00[d]	426.73[d]	127.00	5.53560[p]	496.64[p]
anthracene	$C_{14}H_{10}$	120-12-7	178.23	873.00[d]	29.00[d]	554.00[d]	615.18[d]	213.82	6.77034[p]	675.70[p]
α-pinene	$C_{10}H_{16}$	80-56-8	136.24	632.00[d]	27.60[d]	504.00[d]	429.29[d]	193.64	6.25044[p]	489.17[p]
arachidonic acid (AA)	$C_{20}H_{32}O_2$	506-32-1	304.47	1013.42[e]	12.74[e]	1093.20[e]	819.15[j]	435.92	8.55861[p]	784.39[p]
AA ethyl ester	$C_{22}H_{36}O_2$	1808-26-0	332.53	960.63[a]	11.31[a]	1195.26[a]	777.62[j]	478.66	8.64877[p]	743.53[p]
argon	Ar	7440-37-1	39.95	150.80[b]	48.70[b]	74.90[b]	87.30[b]	26.26	3.40744[q]	123.55[q]
α-tocopherol	$C_{29}H_{50}O_2$	59-02-9	430.71	964.30[h]	10.80[h]	1720.00[h]	787.80[h]	700.94	8.71108[p]	746.37[p]
β-carotene	$C_{40}H_{56}$	7235-40-7	536.88	1450.76[e]	6.90[e]	1934.95[e]	1209.38[j]	793.00	10.08103[s]	1122.89[p]
behenic acid ethyl ester	$C_{24}H_{48}O_2$	5908-87-2	368.64	984.94[a]	9.15[a]	1394.66[a]	806.74[j]	562.66	9.03867[s]	762.34[p]
benzene	C_6H_6	71-43-2	78.11	562.20[b]	48.90[b]	259.00[b]	353.20[b]	96.38	5.19165[q]	308.43[q]
benzoic acid	$C_7H_6O_2$	65-85-0	122.12	752.00[b]	45.60[b]	341.00[b]	523.00[b]	128.58	5.65763[p]	582.05[p]
benzyl acetate	$C_9H_{10}O_2$	140-11-4	150.18	699.00[d]	31.80[d]	449.00[d]	486.65[d]	171.55	6.17454[p]	541.03[p]
benzylacetone	$C_{10}H_{12}O$	2550-26-7	148.20	722.51[f]	31.20[f]	500.50[f]	506.66[l]	192.23	6.27139[p]	559.22[p]
biphenyl	$C_{12}H_{10}$	92-52-4	154.21	789.00[b]	38.50[b]	502.00[b]	529.30[b]	192.83	6.04576[p]	610.69[p]
β-pinene	$C_{10}H_{16}$	127-91-3	136.24	643.00[d]	27.60[d]	506.00[d]	439.19[d]	194.44	6.28262[p]	497.68[p]
bromobenzene	C_6H_5Br	108-86-1	157.01	670.00[b]	45.20[b]	324.00[b]	429.20[b]	121.87	5.47376[p]	518.58[p]
butyric acid ethyl ester	$C_6H_{12}O_2$	105-54-4	116.20	579.00[i]	31.40[i]	400.00[i]	393.15[m]	151.99	5.85491[p]	448.15[p]
caffeine	$C_8H_{10}N_4O_2$	58-08-2	194.20	855.60[i]	41.50[i]	488.00[i]	451.15[m]	187.20	6.05672[p]	662.23[p]
capric acid ethyl ester	$C_{12}H_{24}O_2$	110-38-3	200.00	699.30[i]	17.88[i]	733.50[i]	518.15[m]	286.94	7.28024[p]	541.26[p]
caprylic acid ethyl ester	$C_{10}H_{20}O_2$	106-32-1	172.30	655.70[i]	21.18[i]	621.50[i]	480.15[m]	241.20	6.82453[p]	507.51[p]
carbon dioxide	CO_2	124-38-9	44.01	304.10[b]	73.80[b]	93.90[b]	194.70[d]	33.28	3.26192[q]	500.71[q]
carbon disulphide	CS_2	75-15-0	76.13	552.00[b]	79.00[b]	160.00[b]	319.00[b]	58.18	4.29901[q]	376.51[q]
carbon monoxide	CO	630-08-0	28.01	132.90[b]	35.00[b]	93.20[b]	81.70[b]	33.02	3.53562[p]	102.86[p]
carbon tetrachloride	CCl_4	56-23-5	153.82	556.40[b]	45.60[b]	275.90[b]	349.90[b]	102.98	5.29240[q]	418.84[q]
chlorobenzene	C_6H_5Cl	108-90-7	112.56	632.40[b]	45.20[b]	308.00[b]	404.90[b]	115.57	5.56838[q]	207.50[q]
chlorotrifluoromethane	$CClF_3$	75-72-9	104.46	302.00[b]	38.70[b]	180.40[b]	193.20[b]	65.98	4.37636[q]	410.79[q]
chrysene	$C_{18}H_{12}$	218-01-9	228.29	979.00[d]	23.90[d]	690.00[d]	714.15[d]	269.13	7.37056[p]	757.75[p]
citral	$C_{10}H_{16}O$	5392-40-5	152.24	692.70[e]	23.15[e]	591.00[e]	502.20[n]	228.81	6.75868[p]	536.15[p]
cobalt (III) acetylacetonate	$C_{15}H_{21}CoO_6$	21679-46-9	356.26	573.48[c]	2.52[c]	640.95[c]	411.55[o]	249.11	6.97520[s]	443.87[p]
copper(II) trifluoroacetylacetonate	$C_{10}H_8CuF_6O_4$	14324-82-4	369.70	412.85[c]	20.63[c]	441.13[c]	299.15[k]	168.40	6.00246[p]	319.55[p]
cycloheptanone	$C_7H_{12}O$	502-42-1	112.17	671.19[c]	36.86[c]	297.87[c]	453.15[k]	111.59	5.83247[p]	519.50[p]
cyclohexane	C_6H_{12}	110-82-7	84.16	553.50[b]	40.70[b]	308.00[b]	353.80[b]	115.57	5.73075[q]	224.87[q]
cyclononanone	$C_9H_{16}O$	3350-30-9	140.22	702.10[c]	31.47[c]	380.74[c]	478.25[k]	144.33	6.20206[p]	543.43[p]
cyclopentanone	C_5H_8O	120-92-3	84.12	626.00[d]	58.50[d]	258.00[d]	403.80[d]	95.99	4.94075[p]	484.52[p]
deuterium	D_2	7782-39-0	4.03	38.40[b]	16.50[b]	60.30[b]	23.60[b]	20.92	3.01200[p]	29.72[p]
dibenzo-24-crown-8	$C_{24}H_{32}O_8$	14174-09-5	448.51	1396.77[e]	15.80[e]	1174.35[e]	1111.44[j]	469.89	8.69916[p]	1081.10[p]
dibenzyl ether	$C_{14}H_{14}O$	103-50-4	198.27	777.00[d]	25.60[d]	608.00[d]	561.45[d]	235.71	6.78621[p]	601.40[p]
dicyclohexano-18-crown-6	$C_{20}H_{36}O_6$	16069-36-6	372.50	1177.47[e]	16.24[e]	1002.75[e]	906.84[j]	398.19	8.41774[p]	911.36[p]
dicyclohexano-24-crown-8	$C_{24}H_{44}O_8$	17455-23-1	460.61	1357.66[e]	13.48[e]	1210.75[e]	1077.88[j]	485.16	8.62250[s]	1050.83[p]
diethyl ether	$C_4H_{10}O$	60-29-7	74.12	466.70[b]	36.40[b]	280.00[b]	307.60[b]	104.58	5.23105[p]	361.23[p]
diisopropyl ether	$C_6H_{14}O$	108-20-3	102.18	500.30[b]	28.80[b]	386.00[b]	341.70[b]	146.42	5.74891[p]	387.23[p]
diolein	$C_{39}H_{72}O_5$	2465-32-9	621.99	1025.00[h]	7.92[h]	2150.00[h]	920.00[h]	885.61	10.44146[s]	793.35[p]
D-limonene	$C_{10}H_{16}$	138-86-3	136.24	660.00[d]	27.50[d]	524.00[d]	449.65[d]	201.70	6.33828[p]	510.84[p]
docosahexaenoic acid (DHA)	$C_{22}H_{32}O_2$	6217-54-5	328.49	1075.45[a]	12.41[a]	1148.05[a]	873.23[j]	458.86	8.67455[p]	832.40[p]
DHA ethyl ester	$C_{24}H_{36}O_2$	84494-72-4	356.55	1023.28[a]	10.84[a]	1262.06[a]	831.70[j]	506.73	8.77291[p]	792.02[p]
DHA methyl ester	$C_{23}H_{34}O_2$	28061-46-3	342.52	999.34[a]	11.41[a]	1206.56[a]	808.82[j]	483.40	8.68778[p]	773.49[p]
eicosapentaenoic acid (EPA)	$C_{20}H_{30}O_2$	10417-94-4	302.46	1020.90[a]	13.47[a]	1059.15[a]	823.31[j]	421.70	8.48687[p]	790.18[p]
EPA ethyl ester	$C_{22}H_{34}O_2$	84494-70-2	330.51	968.16[a]	11.67[a]	1173.16[a]	781.78[j]	469.39	8.61744[p]	749.36[p]
EPA methyl ester	$C_{21}H_{32}O_2$	2734-47-6	316.48	890.55[a]	11.90[a]	1187.03[a]	758.90[j]	475.20	8.46741[p]	689.29[p]
ethane	C_2H_6	74-84-0	30.07	305.40[b]	48.80[b]	148.30[b]	184.60[b]	53.73	4.17587[q]	213.99[q]
ethanol	C_2H_6O	64-17-5	46.07	513.90[b]	61.40[b]	167.10[b]	351.40[b]	60.89	4.23738[q]	1291.41[q]

Table 2 (*Continued*)

Substance	Formula	CAS number	M (g/mol)	T_c (K)	P_c (bar)	V_c (cm^3/mol)	T_{bp} (K)	V_{bp}^m (cm^3/mol)	σ_{LJ} (Å)	ε_{LJ}/k_B (K)
ethyl acetate	$C_4H_8O_2$	141-78-6	88.11	523.20[b]	38.30[b]	286.00[b]	350.30[b]	106.93	5.33606[p]	404.96[p]
ethyl benzoate	$C_9H_{10}O_2$	93-89-0	150.18	668.70[b]	23.20[b]	489.00[d]	485.90[b]	187.60	6.68655[p]	517.57[p]
ethylbenzene	C_8H_{10}	100-41-4	106.17	617.20[b]	36.00[b]	374.00[b]	409.30[b]	141.65	5.72572[p]	477.71[p]
ethylene	C_2H_4	74-85-1	28.05	282.40[b]	50.40[b]	130.40[b]	169.30[b]	46.95	4.04838[q]	169.08[q]
ethylferrocene	$C_{12}H_{14}Fe$	1273-89-8	214.09	554.21[c]	27.41[c]	400.64[c]	381.75[o]	152.24	6.02119[p]	428.96[p]
eugenol	$C_{10}H_{12}O_2$	97-53-0	164.20	735.31[f]	33.52[f]	447.23[f]	526.36[l]	170.84	6.17078[p]	569.13[p]
ferrocene	$C_{10}H_{10}Fe$	102-54-5	186.04	786.27[c]	32.07[c]	317.77[c]	522.15[o]	119.42	6.37838[p]	608.57[p]
fluorobenzene	C_6H_5F	462-06-6	96.10	560.10[b]	45.50[b]	269.00[b]	357.90[b]	100.28	5.16448[p]	433.52[p]
γ-linolenic acid	$C_{18}H_{30}O_2$	506-26-3	278.44	958.98[a]	14.17[a]	992.35[a]	769.23[j]	393.87	8.30482[p]	742.25[p]
γ-linolenic acid ethyl ester	$C_{20}H_{34}O_2$	1191-41-9	306.48	937.01[c]	17.56[c]	797.37[c]	663.73[k]	313.17	7.87895[p]	725.25[p]
γ-linolenic acid methyl ester	$C_{19}H_{32}O_2$	301-00-8	292.46	882.79[a]	12.92[a]	1050.86[a]	704.82[j]	418.24	8.32085[p]	683.28[p]
helium	He	7440-59-7	4.00	5.19[b]	2.27[b]	57.40[b]	4.25[b]	19.87	2.99453[p]	4.02[p]
hexachlorobenzene	C_6Cl_6	118-74-1	284.78	825.00[d]	28.50[d]	526.00[d]	582.55[d]	202.51	6.69481[p]	638.55[p]
hydrogen	H_2	1333-74-0	2.02	33.00[b]	12.90[b]	64.30[b]	20.30[b]	22.38	5.94111[q]	3.45E−03[q]
i-butane	C_4H_{10}	75-28-5	58.12	408.20[b]	36.50[b]	263.00[b]	261.40[b]	97.94	5.01034[p]	315.95[p]
indole	C_8H_7N	120-72-9	117.15	790.00[d]	43.00[d]	431.00[d]	526.15[d]	164.35	5.84837[p]	611.46[p]
iodobenzene	C_6H_5I	591-50-4	204.01	721.00[b]	45.20[b]	351.00[b]	461.60[b]	132.53	5.59976[p]	558.05[p]
i-propylbenzene	C_9H_{12}	98-82-8	120.20	631.10[b]	32.10[b]	427.70[d]	425.60[b]	163.03	5.97029[p]	488.47[p]
krypton	Kr	7439-90-9	83.80	209.40[b]	55.00[b]	91.20[b]	119.90[b]	32.28	2.89870[q]	511.92[q]
L-carvone	$C_{10}H_{14}O$	2244-16-8	150.22	709.40[r]	26.30[r]	504.65[r]	507.92[r]	193.90	6.55942[p]	549.08[p]
linalool	$C_{10}H_{18}O$	78-70-6	154.25	645.80[e]	25.95[e]	558.00[e]	472.00[n]	215.44	6.40654[p]	499.85[p]
linoleic acid	$C_{18}H_{32}O_2$	60-33-3	280.45	775.00[h]	14.10[h]	990.00[h]	628.00[h]	392.89	7.93427[p]	599.85[p]
linoleic acid methyl ester	$C_{19}H_{34}O_2$	112-63-0	294.48	870.78[a]	12.54[a]	1070.95[a]	700.66[j]	426.62	8.34769[p]	673.98[p]
L-menthone	$C_{10}H_{18}O$	14073-97-3	154.25	699.44[r]	25.30[r]	525.24[r]	499.40[r]	202.20	6.60650[p]	541.37[p]
methane	CH_4	74-82-8	16.04	190.40[b]	46.00[b]	99.20[b]	111.60[b]	35.25	3.58484[q]	167.15[q]
methanol	CH_4O	67-56-1	32.04	512.60[b]	80.90[b]	118.00[b]	337.70[b]	42.28	3.79957[q]	685.96[q]
methylcyclohexane	C_7H_{14}	108-87-2	98.19	572.20[b]	34.70[b]	368.00[b]	374.10[b]	139.27	5.65749[p]	442.88[p]
monoolein	$C_{21}H_{40}O_4$	111-03-5	356.55	885.00[h]	12.40[h]	1210.00[h]	714.00[h]	484.85	8.39247[p]	684.99[p]
m-xylene	C_8H_{10}	108-38-3	106.17	617.10[b]	35.40[b]	376.00[b]	412.30[b]	142.44	5.75507[p]	477.64[p]
myristic acid ethyl ester	$C_{16}H_{32}O_2$	124-06-1	256.43	789.35[a]	13.89[a]	950.66[a]	623.70[j]	376.54	7.99595[p]	610.96[p]
myristoleic acid	$C_{14}H_{26}O_2$	544-64-9	226.36	854.23[e]	16.97[e]	819.90[e]	669.39[j]	322.45	7.76875[p]	661.17[p]
myristoleic acid methyl ester	$C_{15}H_{28}O_2$	56219-06-8	240.39	777.79[e]	15.26[e]	876.45[e]	604.98[j]	345.80	7.79244[p]	602.01[p]
N-(4-methoxybenzylidene)-4-*n*-butylaniline	$C_{18}H_{21}NO$	26227-73-6	267.37	962.06[c]	21.33[c]	592.93[c]	677.05[k]	229.59	7.55785[p]	744.63[p]
naphthalene	$C_{10}H_8$	91-20-3	128.17	748.40[b]	40.50[b]	413.00[b]	491.10[b]	157.17	5.85874[p]	579.26[p]
n-butane	C_4H_{10}	106-97-8	58.12	425.20[b]	38.00[b]	255.00[b]	272.70[b]	94.82	5.01118[p]	329.10[p]
n-butylbenzene	$C_{10}H_{14}$	104-51-8	134.22	660.50[b]	28.90[b]	497.00[b]	456.50[b]	190.82	6.24687[p]	511.23[p]
n-decane	$C_{10}H_{22}$	124-18-5	142.29	617.70[b]	21.20[b]	603.00[b]	447.30[b]	233.68	6.71395[q]	434.86[q]
n-dodecane	$C_{12}H_{26}$	112-40-3	170.34	658.20[b]	18.20[b]	713.00[b]	489.50[b]	278.54	7.00451[q]	672.90[q]
n-eicosane	$C_{20}H_{42}$	112-95-8	282.56	767.00[b]	11.10[b]	1190.00[d]	617.00[b]	476.45	8.33954[p]	593.66[p]
neon	Ne	7727-37-9	20.18	44.40[b]	27.60[b]	41.60[b]	27.10[b]	14.18	2.66839[p]	34.37[p]
n-heptane	C_7H_{16}	142-82-5	100.21	540.30[b]	27.40[b]	432.00[b]	371.60[b]	164.75	5.94356[q]	404.05[q]
n-hexadecane	$C_{16}H_{34}$	544-76-3	226.45	722.00[b]	14.10[b]	930.00[d]	560.00[b]	367.97	7.36480[q]	1669.19[q]
n-hexane	C_6H_{14}	110-54-3	86.18	507.50[b]	30.10[b]	370.00[b]	341.90[b]	140.06	5.61841[q]	434.76[q]
nitrobenzene	$C_6H_5NO_2$	98-95-3	123.11	719.00[d]	44.00[d]	349.00[d]	483.95[d]	131.74	5.64167[p]	556.51[p]
nitrogen	N_2	7727-37-9	28.01	126.20[b]	33.90[b]	89.80[b]	77.40[b]	31.76	3.51283[p]	97.68[p]
n-nonane	C_9H_{20}	111-84-2	128.26	594.60[b]	22.90[b]	548.00[b]	424.00[b]	211.39	6.43057[q]	497.35[q]
n-octane	C_8H_{18}	111-65-9	114.23	568.80[b]	24.90[b]	492.00[b]	398.80[b]	188.81	6.17328[q]	478.32[q]
n-pentane	C_5H_{12}	109-66-0	72.15	469.70[b]	33.70[b]	304.00[b]	309.20[b]	114.00	5.36967[p]	363.55[p]
n-pentylbenzene	$C_{11}H_{16}$	538-68-1	148.25	679.90[d]	26.04[d]	550.00[d]	478.61[d]	212.20	6.49745[p]	526.24[p]
n-propylbenzene	C_9H_{12}	103-65-1	120.20	638.20[b]	32.00[b]	440.00[b]	432.40[b]	167.95	5.99624[p]	493.97[p]
n-tetradecane	$C_{14}H_{30}$	629-59-4	198.39	693.00[b]	14.40[b]	830.00[b]	526.70[b]	326.62	7.68286[p]	536.38[p]
n-undecane	$C_{11}H_{24}$	1120-21-4	156.31	638.80[b]	19.70[b]	660.00[b]	469.10[b]	256.88	6.91444[p]	494.43[p]
oleic acid	$C_{18}H_{34}O_2$	112-80-1	282.47	781.00[h]	13.90[h]	1000.00[h]	633.00[h]	397.05	7.97503[p]	604.49[p]
oleic acid ethyl ester	$C_{20}H_{38}O_2$	111-62-6	310.52	891.97[e]	11.38[e]	1154.20[e]	719.38[j]	461.44	8.53715[p]	690.38[p]
oleic acid methyl ester	$C_{19}H_{36}O_2$	112-62-9	296.49	868.65[e]	12.01[e]	1098.65[e]	696.50[j]	438.19	8.41384[p]	672.34[p]
oxygen	O_2	7782-44-7	32.00	154.60[b]	50.40[b]	73.40[b]	90.20[b]	25.71	3.29728[p]	119.66[p]
o-xylene	C_8H_{10}	95-47-6	106.17	630.30[b]	37.30[b]	369.00[b]	417.60[b]	139.67	5.70029[p]	487.85[p]

Table 2 (*Continued*)

Substance	Formula	CAS number	M (g/mol)	T_c (K)	P_c (bar)	V_c (cm^3/mol)	T_{bp} (K)	V_{bp}^m (cm^3/mol)	σ_{LJ} (Å)	ε_{LJ}/k_B (K)
palladium(II) acetylacetonate	$C_{10}H_{14}O_4Pd$	14024-61-4	304.64	651.12[c]	4.13[c]	435.41[c]	460.75[o]	166.11	6.13171[s]	503.97[p]
palmitic acid ethyl ester	$C_{18}H_{36}O_2$	628-97-7	284.48	835.62[a]	12.36[a]	1061.66[a]	669.46[j]	422.74	8.30307[p]	646.77[p]
p-dichlorobenzene	$C_6H_4Cl_2$	106-46-7	147.00	684.75[d]	40.70[d]	351.00[d]	447.21[d]	132.53	5.69261[p]	530.00[p]
phenanthrene	$C_{14}H_{10}$	85-01-8	178.23	873.00[b]	29.00[d]	554.00[b]	613.00[b]	213.82	6.77034[p]	675.70[p]
phenol	C_6H_6O	108-95-2	94.11	694.20[b]	61.30[b]	229.00[b]	455.00[b]	84.71	5.03026[p]	537.31[p]
phenylacetic acid	$C_8H_8O_2$	103-82-2	136.15	783.55[e]	38.50[e]	422.60[e]	554.63[j]	161.00	6.03311[p]	606.47[p]
phenylacetylene	C_8H_6	536-74-3	102.14	655.43[d]	44.03[d]	337.50[d]	418.36[d]	127.20	5.48099[p]	507.30[p]
phenylmethanol	C_7H_8O	100-51-6	108.14	720.20[b]	44.00[b]	335.00[d]	478.60[b]	126.21	5.64457[p]	557.43[p]
propane	C_3H_8	74-98-6	44.09	369.80[b]	42.50[b]	203.00[b]	231.10[b]	74.66	4.50412[q]	457.99[q]
p-xylene	C_8H_{10}	106-42-3	106.17	616.20[b]	35.10[b]	379.00[b]	411.50[b]	143.63	5.76754[p]	476.94[p]
pyrene	$C_{16}H_{10}$	129-00-0	202.26	936.00[d]	26.10[d]	630.00[d]	667.95[d]	244.65	7.11077[p]	724.46[p]
squalene	$C_{30}H_{50}$	111-02-4	410.72	974.94[c]	13.23[c]	1128.14[c]	702.45[k]	450.53	8.44342[p]	754.60[p]
stearic acid ethyl ester	$C_{20}H_{40}O_2$	111-61-5	312.54	883.39[a]	11.09[a]	1172.66[a]	715.22[j]	469.18	8.56060[p]	683.74[p]
s-trioxane	$C_3H_6O_3$	110-88-3	90.08	604.00[d]	58.20[d]	206.00[d]	387.65[d]	75.82	4.89292[p]	467.50[p]
styrene	C_8H_8	100-42-5	104.15	647.00[b]	39.90[b]	352.00[d]	418.30[b]	132.93	5.62827[p]	500.78[p]
sulfur hexafluoride	SF_6	2551-62-4	146.05	318.70[b]	37.60[b]	198.80[b]	209.60[b]	73.04	4.76629[q]	271.68[q]
tert-butylbenzene	$C_{10}H_{14}$	98-06-6	134.22	660.00[b]	29.60[b]	492.00[d]	442.30[b]	188.81	6.20099[p]	510.84[p]
tetrabutyltin	$C_{16}H_{36}Sn$	1461-25-2	347.17	767.97[c]	17.25[c]	760.75[c]	548.45[k]	298.12	7.53261[p]	594.41[p]
tetrachloroethene	C_2Cl_4	127-18-4	165.83	620.20[b]	47.60[b]	289.60[b]	394.40[b]	108.35	5.25755[p]	480.03[p]
tetraethyltin	$C_8H_{20}Sn$	597-64-8	234.95	655.92[b]	25.75[b]	429.28[b]	456.25[b]	163.66	6.45057[p]	507.68[p]
tetrafluoromethane	CF_4	75-73-0	88.01	227.60[b]	37.40[b]	139.60[b]	145.10[b]	50.43	4.33323[q]	244.02[q]
tetrahydrofuran	C_4H_8O	109-99-9	72.11	540.10[b]	51.90[b]	224.00[b]	338.00[b]	82.78	4.89719[p]	418.04[p]
tetramethyltin	$C_4H_{12}Sn$	594-27-4	178.85	511.77[c]	34.18[c]	263.54[c]	347.65[k]	98.15	5.49090[p]	396.11[p]
tetrapropyltin	$C_{12}H_{28}Sn$	2176-98-9	291.06	759.88[c]	20.66[c]	595.01[c]	536.35[k]	230.44	7.16016[p]	588.15[p]
thenoyltrifluoroacetone	$C_8H_5F_3O_2S$	326-91-0	222.18	838.69[c]	26.32[c]	428.15[c]	584.42[k]	163.21	6.88052[p]	649.15[p]
toluene	C_7H_8	108-88-3	92.14	591.80[b]	41.00[b]	316.00[b]	383.80[b]	118.72	5.45450[q]	350.74[q]
triarachidonin	$C_{63}H_{98}O_6$	23314-57-0	951.45	1499.66[c]	6.51[c]	2341.53[c]	1135.95[k]	968.46	10.74274[s]	1160.74[p]
trierucin	$C_{69}H_{128}O_6$	2752-99-0	1053.75	1549.28[c]	5.62[c]	2832.93[c]	1182.75[k]	1182.46	11.44706[s]	1199.14[p]
trifluoroacetylacetone	$C_5H_5F_3O_2$	367-57-7	154.09	594.02[a]	32.89[a]	365.58[a]	416.12[j]	138.31	5.81789[p]	459.77[p]
trinervonin	$C_{75}H_{140}O_6$	81913-24-8	1137.91	1601.10[c]	5.20[c]	3081.54[c]	1229.05[k]	1291.44	11.77257[s]	1239.25[p]
triolein	$C_{57}H_{104}O_6$	122-32-7	885.43	1448.04[c]	6.70[c]	2335.72[c]	1091.85[k]	965.94	10.73385[s]	1120.75[p]
ubiquinone CoQ10	$C_{59}H_{90}O_4$	303-98-0	863.34	1522.50[c]	7.09[c]	2146.17[c]	1142.15[k]	883.95	10.43526[s]	1178.42[p]
vanillin	$C_8H_8O_3$	121-33-5	152.15	777.00[d]	40.10[d]	415.00[d]	558.00[d]	157.96	5.94398[p]	601.40[p]
vitamin K_1	$C_{31}H_{48}O_2$	84-80-0	452.71	1329.54[e]	8.58[e]	1620.20[e]	1099.02[j]	658.37	9.50177[s]	1029.06[p]
vitamin K_3	$C_{11}H_8O_2$	58-27-5	172.18	893.85[e]	31.96[e]	537.20[e]	638.20[j]	207.03	6.62868[p]	691.84[p]
xenon	Xe	7440-63-3	131.30	289.70[b]	58.40[b]	118.40[b]	165.00[b]	42.43	3.85754[p]	224.23[p]

[a]Average of the values by the Joback [13,49,50] and Somayajulu [51] methods. [b]Taken from Reid et al. [13]. [c] Estimated by the Klincewicz [13,52] method. [d]Taken from Yaws [149]. [e]Average of the values by the Joback [13,49] and Ambrose [13,53,54] methods. [f]Average of the values by the Joback [13,49,50] and Wen-Qiang [55] methods. [g]Taken from Korea Thermophysical Properties Data Bank (KDB) [150]. [h]Taken from ASPEN database [151]. [i]Taken from Table 4 of Liu and Ruckenstein [152]. [j]Estimated by the Joback [13,49,50] method. [k]Taken from ChemSpider [153]. [l]Taken from Lide [154]. [m]Estimated by the Tyn-Calus [13,48] expression. [n]Taken from Green and Perry [155]. [o]Taken from LookChem [156]. [p]Estimated by Eqs. (14) and (15) whenever $T_c/P_c < 100$. [q]Taken from Table 7 of Liu et al. [32]. [r]Average of the values by the Joback [13,49,50] and Constantinou-Gani [56] methods. [s]Estimated by $\sigma_{LJ} = 0.809V_c^{1/3}$, since $T_c/P_c > 100$.

Table 3
Calculated results (note: an hyphen means is not applicable).

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s $K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
					Supercritical systems						
2,3-dimethylbutane	benzene	11	11.6929	1.34	0.9661	70.08	1.56	7.93	75.95	95.80	44.77
	naphthalene	9	13.0408	1.40	0.7527	66.74	1.75	2.41	65.82	82.61	60.31
	phenanthrene	11	12.3225	1.91	0.5871	54.23	1.53	5.23	61.35	78.84	72.56
	toluene	10	11.9749	1.30	0.9458	77.91	1.79	4.82	72.49	90.48	51.73
carbon dioxide	1,1,1,5,5,5-hexafluoroacetylacetone	15	11.6230	4.36	1.1460	11.05	4.36	23.39	18.95	39.26	32.24
	1,1′-dimethylferrocene	68	10.6896	2.39	1.2835	11.85	3.67	29.12	12.16	31.02	18.70
	1,2-dichlorobenzene	15	9.0441	1.75	1.5427	16.61	2.07	10.51	6.89	22.17	17.55
	1,2-diethylbenzene	15	8.4807	1.99	1.3663	15.06	2.61	11.78	6.19	14.43	17.28
	1,3,5-trimethylbenzene	24	10.0258	4.60	1.2531	11.01	4.29	13.33	7.27	23.55	19.18
	1,3-divinylbenzene	15	7.7970	1.20	1.5589	18.35	1.39	12.10	3.74	16.70	16.58
	1,4-diethylbenzene	15	8.4584	2.66	1.3865	15.72	4.06	11.17	5.65	15.36	18.05
	15-crown-5	29	6.9828	5.84	0.9986	1.19	5.98	21.17	7.85	21.59	15.09
	1-naphthol	11	5.8650	2.56	2.1460	24.53	0.88	9.22	5.77	9.17	4.60
	1-phenyldodecane	15	11.1646	2.43	0.9485	17.21	3.14	26.54	6.96	27.70	47.18
	1-phenylethanol	15	12.1262	1.70	1.3428	14.22	3.15	11.15	10.31	28.54	25.33
	1-phenylhexane	15	8.6859	2.03	1.2534	16.08	2.71	14.59	7.52	16.20	23.78
	1-phenyloctane	15	8.0059	2.72	1.1894	16.53	3.65	20.79	8.65	16.88	27.35
	1-propanol	17	9.3807	4.61	1.3448	-10.04	3.00	8.71	15.43	26.25	4.49
	2,2,4,4-tetramethyl-3-pentanone	9	-1.2255	2.90	3.0352	29.08	0.76	24.62	27.01	14.50	20.80
	2,3-dimethylaniline	15	12.2897	2.19	1.2259	13.77	2.38	12.08	16.04	35.59	33.42
	2,3-dimethylnaphthalene	3	8.0571	1.18	1.5361	21.43	1.08	10.35	3.66	16.99	18.98
	2,4-dimethyl-3-pentanone	8	12.2269	3.28	1.7583	25.46	2.33	27.67	29.97	47.89	28.35
	2,4-dimethylphenol	15	12.5119	2.87	1.1649	8.33	3.63	11.95	9.42	27.40	24.55
	2,6-dimethylaniline	15	12.7114	3.12	1.1330	8.66	3.34	11.78	11.47	30.25	28.06
	2,6-dimethylnaphthalene	6	8.6630	4.33	1.1736	10.78	4.24	15.38	7.15	17.98	18.68
	2,7-dimethylnaphthalene	6	7.7956	4.50	1.5069	19.63	4.50	11.91	6.91	13.01	16.04
	2-bromoanisole	15	11.4509	2.26	1.2561	12.79	3.66	10.23	16.52	35.12	30.69
	2-butanone	38	6.2891	1.96	2.0672	16.91	2.60	9.83	5.38	7.75	4.85
	2-ethyltoluene	15	8.4941	3.30	1.4172	14.72	3.76	9.30	8.95	9.76	10.53
	2-fluoroanisole	15	10.9097	1.71	1.3944	14.19	2.58	9.93	18.48	35.01	26.66
	2-heptanone	11	0.0071	4.68	3.4792	32.29	1.83	22.02	30.11	17.77	23.07
	2-methylanisole	15	10.5104	2.18	1.3055	12.12	2.79	9.69	9.67	26.90	22.89
	2-naphthol	16	4.8419	4.19	1.9948	21.27	1.73	6.52	7.84	7.67	10.71
	2-nitroanisole	15	11.2230	1.73	1.2984	15.75	2.39	10.88	11.47	31.20	30.58
	2-nonanone	10	−2.5576	3.86	2.8331	29.00	2.35	25.05	35.76	21.43	25.20
	2-pentanone	23	6.2588	1.98	1.7185	12.62	2.52	7.78	4.45	12.64	2.27
	2-phenyl-1-propanol	15	13.1297	1.70	1.2825	15.24	2.64	15.83	9.72	30.05	30.05
	2-phenylethanol	15	11.8008	1.90	1.3652	15.18	3.03	10.31	12.10	30.39	26.79
	2-phenylethyl acetate	15	12.3946	2.52	1.1080	13.22	3.06	13.89	8.63	32.02	36.37
	2-propanol	18	7.0638	3.70	1.5735	-1.37	2.21	7.42	9.57	19.89	7.64
	3-ethyltoluene	15	8.1446	3.59	1.4175	14.91	4.00	9.82	11.68	7.07	9.09
	3-nitrotoluene	15	9.9120	2.56	1.3849	14.90	3.96	9.58	4.00	17.91	18.41
	3-pentanone	39	6.1599	1.62	2.0419	19.27	2.03	9.04	9.48	4.37	4.31
	3-phenyl-1-propanol	15	11.8564	1.85	1.5158	20.64	2.28	9.50	6.21	26.32	27.20
	3-phenylpropyl acetate	15	12.2121	2.99	1.0565	12.96	3.37	14.86	7.12	31.18	38.05
	4-ethyltoluene	15	9.0303	2.81	1.4780	17.40	3.07	8.89	7.46	11.41	12.72
	4-heptanone	9	−3.1193	2.12	3.1752	27.31	0.47	29.62	36.53	25.01	29.68
	4-methylanisole	15	12.2670	2.06	1.3473	16.11	3.21	12.16	17.52	35.98	31.81
	5-nonanone	12	−1.7755	4.82	3.0575	32.15	1.10	25.83	34.31	19.33	20.80
	5-*tert*-butyl-*m*-xylene	31	8.2774	1.74	1.6033	22.88	3.02	13.60	8.45	14.08	19.41
	6-undecanone	13	−2.1381	4.55	2.8101	31.76	2.53	27.76	38.53	21.79	20.74

Table 3 (*Continued*)

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s $K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
	acetone	178	7.6727	4.34	2.1316	13.74	5.05	11.71	5.64	12.59	10.29
	acridine	6	10.0396	2.64	1.2634	16.55	2.85	15.47	4.93	20.98	27.22
	adamantanone	8	−1.7883	2.59	1.4379	-2.78	2.59	29.47	18.17	7.13	14.95
	α-linolenic acid	56	8.9849	3.53	0.9745	15.74	2.79	26.31	14.24	18.39	32.29
	allylbenzene	15	9.2397	3.35	1.3060	10.81	3.34	10.60	5.36	17.71	16.32
	aniline	15	15.1453	3.04	1.1791	8.61	2.46	21.45	33.34	48.89	33.65
	anisole	15	10.3116	1.99	1.4822	13.90	2.97	7.70	7.33	22.66	16.31
	anthracene	22	5.3986	2.71	1.6433	22.35	1.75	20.69	10.38	9.98	14.67
	α-pinene	15	7.4629	3.67	1.7055	21.73	3.83	9.38	7.00	12.54	9.28
	arachidonic acid (AA)	75	7.3558	5.03	0.8591	13.44	2.51	49.72	9.70	25.84	41.11
	AA ethyl ester	48	6.6406	0.58	1.1233	23.26	1.17	37.41	15.16	19.76	30.43
	α-tocopherol	82	6.8389	2.86	0.9419	18.16	2.21	64.17	31.55	4.98	27.17
	β-carotene	90	7.9366	3.75	0.6748	16.79	2.26	144.58	14.88	33.25	66.19
	behenic acid ethyl ester	17	5.3588	1.21	1.2263	27.32	0.86	65.88	21.34	14.66	31.30
	benzene	222	5.9164	7.57	1.4921	-1.03	7.59	11.77	9.14	11.09	9.70
	benzoic acid	29	8.9295	5.81	1.8170	21.69	6.34	8.54	9.27	23.35	14.24
	benzyl acetate	15	10.4248	2.11	1.3600	16.99	3.02	9.82	7.79	27.69	28.09
	benzylacetone	15	11.1435	2.67	1.0795	9.68	3.76	12.63	6.19	27.48	30.46
	biphenyl	24	8.4650	3.58	1.3557	13.85	3.39	15.21	10.13	10.78	10.04
	β-pinene	15	5.8642	3.51	1.3716	9.22	4.97	10.14	11.72	7.30	5.08
	bromobenzene	15	10.2376	4.62	1.4373	12.25	4.36	9.08	7.81	21.50	13.52
	butyric acid ethyl ester	16	7.2422	3.51	2.2177	27.36	1.89	3.91	4.31	11.80	6.58
	caffeine	21	14.0214	7.74	0.7164	-17.53	4.87	37.00	22.62	47.40	31.48
	capric acid ethyl ester	16	6.1850	2.82	1.7729	29.09	1.44	10.56	13.46	11.25	16.75
	caprylic acid ethyl ester	16	6.9489	2.19	1.7619	26.83	1.67	7.39	10.23	12.15	14.33
	chlorobenzene	15	10.5647	3.84	1.4476	11.52	3.61	8.91	8.22	21.67	12.35
	chrysene	4	4.0191	1.89	1.8594	27.80	2.61	43.90	16.16	6.63	18.17
	citral	15	6.6552	2.94	1.3860	16.29	4.31	10.55	8.63	13.20	11.19
	cobalt(III) acetylacetonate	38	12.8945	1.49	1.0715	17.87	2.13	125.95	11.53	40.06	47.22
	copper(II) trifluoroacetylacetonate	12	17.1980	4.48	1.2764	22.66	5.04	72.60	37.09	62.37	52.90
	cycloheptanone	8	8.7825	2.90	1.8569	23.71	1.85	8.58	24.01	39.72	18.83
	cyclononanone	8	9.0682	3.10	1.7583	25.46	2.33	10.68	17.62	36.52	22.69
	cyclopentanone	8	11.3711	1.30	1.8382	18.40	1.03	13.18	20.31	33.53	9.61
	dibenzo-24-crown-8	28	6.9846	1.72	1.0944	24.24	1.93	99.02	12.73	22.77	51.41
	dibenzyl ether	15	10.8917	2.62	1.0702	14.04	3.22	15.81	5.32	30.14	38.16
	diethyl ether	15	10.4661	14.48	1.0474	-26.59	4.98	32.29	11.80	22.80	9.09
	diisopropyl ether	15	8.5982	10.04	1.0782	-16.29	7.87	29.92	7.14	12.53	11.51
	diolein	9	5.7684	4.81	0.6769	14.02	1.61	77.97	23.69	22.33	48.58
	D-limonene	15	6.9199	3.29	1.3735	12.04	4.06	10.49	9.32	10.54	7.22
	docosahexaenoic acid (DHA)	63	8.1947	2.87	0.9162	18.60	1.63	58.53	7.28	30.05	48.35
	DHA ethyl ester	65	6.4044	1.10	1.0708	22.09	1.45	48.46	16.73	18.88	31.39
	DHA methyl ester	17	6.0194	0.86	1.2079	25.70	0.92	52.38	16.76	17.74	32.12
	eicosapentaenoic acid (EPA)	55	7.6249	3.48	0.9184	16.15	1.79	46.01	7.79	27.28	41.67
	EPA ethyl ester	48	6.5200	0.68	1.1626	24.23	1.06	36.48	14.98	19.58	29.92
	EPA methyl ester	17	6.6928	1.40	1.2964	27.43	0.49	37.76	17.37	16.49	30.48
	ethanol	24	8.0520	2.98	1.9621	6.43	3.21	12.41	11.29	19.52	9.68
	ethyl acetate	15	10.4849	17.12	0.8254	-49.61	6.71	36.32	12.75	24.58	8.21
	ethyl benzoate	15	7.3630	4.55	1.8993	27.23	2.94	12.20	3.88	22.01	24.86
	ethylbenzene	15	7.1995	1.83	1.8248	18.85	2.28	9.47	7.44	7.97	4.84
	eugenol	15	12.5981	2.90	1.3885	20.62	3.58	10.54	17.29	39.19	39.69
	ferrocene	98	5.4911	3.40	1.2424	6.91	6.35	21.24	17.32	33.15	18.19
	fluorobenzene	15	10.8771	3.61	1.7808	17.76	4.22	10.40	11.04	23.76	10.83
	γ-linolenic acid	142	7.5649	5.23	0.8364	9.15	2.15	33.37	7.79	26.40	36.36
	γ-linolenic acid ethyl ester	41	9.9816	6.34	0.8603	6.15	5.10	43.72	6.92	37.84	23.99

Table 3 (*Continued*)

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s $K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
	γ-linolenic acid methyl ester	52	7.4397	6.33	0.8588	7.53	7.58	47.11	13.41	19.17	19.94
	hexachlorobenzene	14	6.7978	8.55	0.8331	-12.47	4.18	25.04	10.99	20.34	14.18
	iodobenzene	15	11.9409	3.14	1.2680	11.18	2.72	11.69	12.21	28.89	22.56
	i-propylbenzene	15	7.1693	2.16	1.6274	17.00	2.00	10.94	9.27	7.60	7.33
	L-carvone	23	8.4989	3.18	1.6268	23.50	2.57	11.23	3.95	21.17	24.19
	linalool	15	8.0284	3.27	1.3508	14.09	4.02	11.26	7.24	13.86	10.49
	linoleic acid	71	9.4472	5.66	0.8351	9.74	3.73	30.68	9.63	25.29	38.00
	linoleic acid methyl ester	21	6.3307	2.23	1.0645	19.77	1.66	56.92	15.74	16.35	37.24
	L-menthone	23	7.5505	3.56	1.7676	25.22	2.81	11.73	5.18	15.93	19.79
	methanol	10	8.0885	3.97	2.1980	1.60	2.14	20.87	16.79	23.92	18.17
	monoolein	11	9.9118	3.58	0.8199	13.88	1.22	24.17	8.71	29.20	43.52
	myristic acid ethyl ester	16	5.8944	2.42	1.4546	27.11	2.14	24.88	15.97	13.35	23.65
	myristoleic acid	42	9.3432	5.62	0.8465	4.77	2.66	25.97	5.68	32.51	31.43
	myristoleic acid methyl ester	79	11.0829	8.88	0.7247	-15.38	10.07	68.29	10.41	29.12	14.33
	N-(4-methoxybenzylidene)-4-*n*-butylaniline	5	−0.5082	1.26	2.1419	29.00	0.33	42.04	17.85	1.84	3.72
	naphthalene	83	7.9398	8.46	1.4146	11.79	8.29	18.59	10.81	14.62	10.14
	n-butylbenzene	15	8.4175	1.94	1.4109	15.95	2.97	11.18	6.29	13.93	16.57
	n-decane	5	−1.9772	4.28	3.8443	36.48	1.47	32.31	38.51	23.56	21.11
	n-dodecane	5	−2.4436	6.38	4.3507	39.93	2.99	37.54	40.87	24.36	19.59
	n-heptane	5	1.0716	3.79	3.9421	35.67	1.00	20.99	28.91	16.05	18.71
	n-hexane	5	2.6677	3.64	3.9838	35.55	2.09	16.06	22.91	10.85	16.44
	nitrobenzene	15	10.2898	2.18	1.2975	9.79	3.33	9.96	8.79	24.87	19.22
	n-nonane	5	−1.1931	4.42	4.0604	37.02	1.43	29.33	36.45	22.22	21.11
	n-octane	5	−0.1518	4.51	4.1527	37.05	1.66	25.60	33.41	19.86	20.36
	n-pentane	5	4.5108	4.00	4.0586	35.82	1.67	9.12	13.23	2.52	12.10
	n-pentylbenzene	31	8.3397	1.94	1.6168	21.86	3.95	12.96	8.27	13.58	17.27
	n-propylbenzene	34	9.0653	9.49	0.8647	-17.49	5.03	25.18	12.75	20.46	8.67
	n-tetradecane	5	−2.4383	7.65	4.3703	41.99	3.32	43.05	38.78	19.50	12.24
	n-undecane	5	−2.8335	5.24	4.1553	38.28	1.85	35.87	40.94	25.46	21.81
	oleic acid	19	9.5105	5.85	0.8088	9.94	2.14	37.36	10.03	26.11	40.02
	oleic acid ethyl ester	5	11.0841	7.85	0.5458	-23.03	0.97	53.72	5.72	38.56	29.14
	oleic acid methyl ester	19	12.2814	8.17	0.5031	-34.23	1.93	65.15	6.50	42.07	27.79
	palladium(II) acetylacetonate	125	13.24401	2.36	1.2460	17.11	4.65	91.51	21.93	44.15	38.05
	palmitic acid ethyl ester	17	6.4017	1.27	1.3142	26.47	0.61	30.82	15.14	16.97	28.90
	p-dichlorobenzene	13	9.6489	3.59	1.5067	16.27	3.72	8.76	10.61	27.05	17.02
	phenanthrene	19	3.9920	6.18	1.3448	12.04	5.03	23.94	13.96	8.79	6.02
	phenol	109	9.6578	3.01	1.3641	2.62	4.61	8.02	21.47	33.35	10.35
	phenylacetic acid	16	8.8548	1.90	1.7122	22.71	1.80	6.41	4.25	22.72	15.84
	phenylacetylene	15	10.4016	1.13	1.6377	17.26	1.58	7.61	7.80	22.91	16.04
	phenylmethanol	15	10.5980	1.61	1.5257	16.57	2.54	8.05	13.91	30.10	22.63
	pyrene	18	5.9952	2.50	1.5497	23.47	1.84	26.23	9.18	13.72	20.83
	squalene	5	7.0990	4.18	1.9069	36.68	1.87	50.04	13.56	20.60	38.21
	stearic acid ethyl ester	17	6.4240	1.32	1.2474	26.37	1.03	41.53	16.25	17.77	31.65
	styrene	15	10.6398	4.00	1.6454	18.93	4.39	8.35	5.38	20.35	14.72
	tert-butylbenzene	15	8.2675	3.73	1.8018	23.59	3.62	9.25	7.92	10.83	14.03
	tetrahydrofuran	15	10.1526	12.53	1.1871	-22.18	4.99	22.16	15.96	27.07	10.90
	thenoyltrifluoroacetone	15	9.9795	3.61	1.1938	18.09	3.05	13.70	30.20	53.55	47.64
	toluene	35	7.2441	4.06	1.6490	11.46	4.14	8.44	5.32	11.84	4.46
	triarachidonin	27	7.7442	8.26	0.4912	6.85	0.82	149.23	17.49	34.89	70.26
	trierucin	101	9.6030	9.64	0.3731	-2.73	2.95	146.62	13.57	48.33	82.31
	trifluoroacetylacetone	15	7.9615	1.83	1.7229	19.57	2.18	6.36	3.74	19.21	11.17
	trinervonin	38	8.6611	8.67	0.3962	2.77	2.86	163.95	16.62	45.38	83.21
	triolein	10	9.8300	7.64	0.4442	-1.58	1.26	100.27	11.80	44.11	66.59
	ubiquinone CoQ10	80	8.6671	5.04	0.6220	16.09	4.09	141.53	13.90	37.98	71.55

Table 3 (*Continued*)

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s $K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
	vanillin	15	11.0112	1.87	1.5345	21.13	2.03	10.92	12.64	32.26	24.63
	vitamin K_1	16	3.4907	4.00	0.8940	16.80	2.22	106.89	27.19	9.60	30.62
	vitamin K_3	20	6.2302	4.51	1.1807	8.84	2.70	24.21	9.77	12.90	11.31
chlorotrifluoromethane	acetone	10	12.4127	6.13	0.9096	19.58	2.56	5.85	23.27	25.58	23.11
	p-xylene	8	14.5514	11.17	0.4851	-13.32	2.28	38.21	23.77	21.94	31.30
ethane	1-octene	6	6.1933	5.90	1.2050	12.75	1.40	11.82	4.78	54.05	4.19
	1-tetradecene	9	2.8288	2.30	1.5925	38.24	1.61	18.87	17.61	37.37	5.15
sulfur hexafluoride	1,3,5-trimethylbenzene	10	9.0490	9.65	0.5377	18.96	4.59	14.17	33.06	45.23	32.11
	benzene	9	7.8833	9.07	0.6679	1.44	10.58	7.33	39.39	47.80	40.59
	benzoic acid	6	11.9344	4.58	0.6061	40.87	2.61	17.30	149.89	81.32	165.45
	carbon tetrachloride	6	8.8200	2.57	0.6877	35.40	5.18	13.73	37.99	32.10	50.14
	naphthalene	5	4.2289	6.03	1.1687	67.42	5.52	11.07	77.19	30.05	111.97
	p-xylene	52	6.1192	7.19	0.5781	19.73	12.41	7.75	23.28	40.99	34.37
	toluene	11	8.7644	10.84	0.5288	-18.56	9.73	7.21	37.76	49.77	35.50
					Liquid systems						
2,2,4-trimethylpentane	1,3,5-trimethylbenzene	4	18.3560	2.74	1.0142	150.50	0.84	36.05	58.70	63.87	176.33
	benzene	4	14.3556	1.57	1.1336	145.53	1.61	26.78	48.72	57.73	116.69
	ethylbenzene	4	17.2713	1.55	0.8035	144.09	1.33	35.01	55.63	61.41	157.33
	o-xylene	4	16.4807	2.39	0.9929	147.66	2.24	29.54	51.64	57.35	149.74
	p-xylene	4	13.5319	2.84	0.7954	140.69	1.94	17.09	35.18	40.13	124.47
	toluene	4	14.5635	1.61	1.0099	144.99	1.58	23.72	43.53	50.09	123.97
cyclohexane	1,1′-dimethylferrocene	5	13.0504	6.63	0.5416	98.23	5.36	219.79	28.45	37.44	191.46
	1,3,5-trimethylbenzene	12	4.2229	11.78	1.1194	101.54	2.42	56.15	26.15	24.98	74.04
	argon	6	-0.4301	6.03	2.6698	96.95	2.44	43.30	21.29	4.19	14.01
	benzene	12	3.4685	8.89	1.4520	101.34	3.04	66.34	25.76	25.20	61.82
	carbon tetrachloride	6	5.5469	5.45	1.3613	102.47	1.11	76.72	6.41	4.69	61.75
	ethane	5	0.8264	7.55	2.0214	100.00	2.40	106.17	25.57	17.12	19.02
	ethylene	5	0.8145	9.28	2.1435	99.75	2.30	102.01	25.19	15.54	14.29
	ethylferrocene	6	12.2874	5.98	0.5775	99.11	5.21	191.79	29.02	38.05	193.21
	ferrocene	5	7.4065	6.67	0.5481	97.15	5.52	71.02	35.44	44.73	183.7
	krypton	6	7.7648	6.00	2.1405	98.04	1.26	66.64	8.49	9.36	8.06
	methane	6	4.3374	4.43	2.8585	99.81	0.68	40.39	28.46	16.26	13.59
	naphthalene	12	3.3398	11.63	1.1611	101.24	2.99	40.63	26.63	24.61	69.07
	phenanthrene	8	4.5913	10.49	0.9775	101.00	4.31	6.34	39.49	34.47	47.00
	p-xylene	8	3.4651	12.40	1.2210	100.22	3.88	28.73	40.98	36.91	37.42
	tetrabutyltin	7	10.9921	6.98	0.7438	103.12	2.35	13.61	6.48	8.50	145.59
	tetraethyltin	7	6.2492	7.33	1.0441	102.93	2.16	57.13	5.80	6.36	101.58
	tetramethyltin	7	5.3872	8.22	1.2553	102.25	1.25	94.10	4.80	10.31	81.47
	tetrapropyltin	6	7.7236	7.97	0.8573	102.94	2.10	21.82	4.89	7.53	129.86
	toluene	12	2.6425	11.38	1.3305	100.99	2.85	55.83	26.14	24.07	59.85
	xenon	6	3.6475	10.18	1.8186	99.39	1.15	85.28	5.62	13.76	25.48
n-decane	12-crown-4	4	14.9215	4.33	0.5689	183.45	2.87	40.09	24.21	24.33	174.46
	15-crown-5	4	16.2075	7.28	0.4514	182.06	5.22	22.23	28.12	27.29	204.00
	18-crown-6	4	16.8132	3.78	0.4654	184.73	3.14	4.80	28.17	27.06	224.00
	argon	3	11.9514	0.79	1.8070	179.89	0.32	47.60	3.65	28.17	15.91
	carbon tetrachloride	3	12.3033	2.64	0.7923	183.18	0.14	71.32	17.93	22.49	122.24
	dicyclohexano-18-crown-6	4	18.8529	1.80	0.3810	185.79	1.16	84.24	27.03	27.14	272.75
	dicyclohexano-24-crown-8	4	18.8549	1.80	0.3344	185.84	1.71	137.91	29.14	30.64	304.55

Table 3 (*Continued*)

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s $K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
	krypton	3	19.0725	0.39	1.3923	180.80	0.78	69.75	16.32	45.82	45.72
	methane	3	17.5992	0.91	1.8223	181.67	0.03	46.00	12.44	7.71	18.52
	s-trioxane	4	13.2383	2.37	0.8812	182.90	0.42	50.22	25.93	35.61	112.93
	tetrabutyltin	4	19.3337	6.66	0.4353	185.39	2.16	20.57	23.40	22.46	216.69
	tetraethyltin	3	13.7937	6.62	0.5949	183.97	1.42	47.46	19.59	19.92	157.62
	tetramethyltin	4	14.0521	5.56	0.7287	183.47	1.43	71.35	30.51	36.23	131.15
	tetrapropyltin	4	16.6352	6.66	0.4903	184.67	1.55	24.65	23.25	22.27	190.08
	xenon	4	13.5149	2.14	1.1823	181.74	0.62	68.96	23.29	46.08	65.08
n-dodecane	1,3,5-trimethylbenzene	4	15.1196	2.09	0.4609	213.97	0.79	119.21	16.71	13.20	206.98
	acetone	5	17.4902	1.19	0.8244	215.52	1.68	102.53	16.62	23.08	133.34
	benzene	4	15.2967	0.79	0.6766	214.82	1.30	122.54	16.31	18.96	156.36
	carbon dioxide	9	17.7949	3.09	1.2167	210.03	2.20	23.83	10.06	18.79	17.40
	carbon monoxide	9	18.0846	7.20	1.4392	212.70	5.90	27.26	17.45	16.32	13.29
	hydrogen	9	34.2553	6.57	3.9660	215.14	5.29	47.80	59.75	44.93	59.39
	linoleic acid methyl ester	4	20.7100	0.53	0.2853	217.39	0.92	41.86	13.66	8.50	335.44
	m-xylene	4	13.4291	1.43	0.5477	214.25	1.54	108.51	9.33	7.60	173.92
	naphthalene	5	13.7023	2.07	0.5064	214.04	1.41	81.24	12.27	9.28	183.79
	n-decane	5	13.1427	6.85	0.5822	219.24	2.98	29.97	21.54	25.19	80.95
	n-hexadecane	5	18.3101	6.69	0.4466	221.99	6.69	19.30	14.84	19.00	130.15
	n-octane	9	12.9556	4.16	0.6640	218.97	1.48	25.45	21.35	24.34	62.05
	n-tetradecane	5	15.1250	8.76	0.4729	221.14	7.84	17.19	18.00	20.79	114.67
	toluene	4	14.0054	1.47	0.6374	214.93	2.01	110.79	9.90	9.70	159.39
n-eicosane	carbon dioxide	5	30.6951	2.07	0.8724	352.03	2.07	21.16	16.80	21.39	28.22
	carbon monoxide	5	32.4152	2.39	1.0324	354.30	2.43	31.74	19.36	15.23	13.28
	hydrogen	5	53.2444	4.04	3.0212	357.65	4.65	36.80	62.00	45.86	54.06
	n-dodecane	5	23.6796	4.55	0.3222	361.84	4.28	60.70	14.60	25.27	139.25
	n-hexadecane	5	25.7495	5.52	0.2678	362.04	3.44	55.72	13.47	24.58	169.03
	n-octane	5	22.6581	4.66	0.4003	359.67	4.78	56.15	16.80	24.94	103.21
n-heptane	*n*-decane	5	10.7932	3.19	0.9631	132.45	1.65	6.81	34.06	28.81	36.75
	n-dodecane	5	11.1033	3.08	0.8855	132.67	2.18	15.55	30.61	24.63	55.32
	n-hexadecane	8	14.0921	3.15	0.7499	133.82	3.09	24.56	33.68	26.86	57.37
	n-octane	4	9.7681	2.45	1.1427	133.32	1.92	5.00	35.23	30.29	31.76
	n-tetradecane	5	11.2144	3.13	0.8028	133.05	2.96	29.65	29.40	22.68	64.30
n-hexadecane	carbon dioxide	10	31.0751	3.56	0.9379	278.97	1.91	34.82	12.21	24.25	24.16
	carbon monoxide	10	32.9237	3.06	1.0499	280.25	3.08	51.49	13.21	18.74	15.71
	hydrogen	10	50.3284	13.34	2.1314	268.40	7.32	37.24	55.28	38.35	49.80
	n-decane	5	25.6504	5.73	0.4751	291.18	6.01	62.45	13.07	19.99	116.34
	n-dodecane	5	25.8228	3.05	0.3976	288.61	2.43	55.76	14.96	20.42	127.81
	n-octane	10	25.5133	5.77	0.5159	289.46	3.65	64.04	13.88	19.16	100.91
	n-tetradecane	5	25.2249	3.73	0.3774	290.23	5.42	42.01	13.59	21.15	139.97
n-hexane	1,1′-dimethylferrocene	4	19.6538	5.75	0.1282	-0.01	5.76	57.06	19.62	32.93	109.75
	1,3,5-trimethylbenzene	20	12.4970	4.18	0.8743	101.17	14.54	5.88	48.09	46.33	52.86
	acetone	5	11.3525	2.74	1.4801	111.01	3.03	7.37	5.42	20.34	47.08
	acetonitrile	7	10.1549	5.17	1.1551	102.14	5.93	22.16	115.32	146.30	185.38
	benzene	36	9.8172	6.68	1.1371	103.51	14.54	26.17	80.10	88.03	121.67
	carbon disulphide	10	6.4817	6.22	1.1409	102.23	4.66	64.04	178.18	224.06	262.41
	ethylferrocene	4	19.2030	5.56	0.1264	-0.01	5.70	45.98	21.26	34.76	112.64
	ferrocene	4	14.6000	5.37	0.1382	-0.01	5.47	8.76	28.28	43.09	107.67

Table 3 (*Continued*)

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s $K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
	indole	4	11.7688	4.11	0.4384	84.37	2.83	10.84	10.40	1.82	64.47
	m-xylene	5	11.5153	2.71	1.3601	115.15	2.00	5.49	6.24	11.14	70.80
	naphthalene	20	11.1684	5.43	0.8828	98.35	15.15	10.14	49.57	46.00	49.62
	phenanthrene	15	10.8404	5.07	0.6767	81.65	11.81	12.83	63.76	59.51	42.96
	p-xylene	17	11.2087	5.76	0.9088	93.68	16.35	8.34	56.45	54.22	49.73
	toluene	28	9.7194	6.71	1.0354	102.80	16.17	18.14	78.86	85.17	126.71
n-octane	1,3,5-trimethylbenzene	4	13.7859	0.99	0.8117	148.56	0.28	22.30	8.13	13.36	116.12
	argon	4	10.9264	1.78	1.9181	142.44	2.94	19.90	2.39	32.43	9.41
	benzene	4	9.6781	2.17	1.0124	144.89	0.22	16.11	0.98	7.81	66.99
	carbon tetrachloride	4	12.5805	1.54	1.0157	148.85	0.59	34.74	12.51	20.88	89.67
	ethyl benzene	4	12.7658	2.95	0.7797	145.55	1.55	22.88	6.06	11.77	101.41
	krypton	4	17.5478	1.56	1.5181	143.52	2.86	37.40	16.13	46.81	28.78
	methane	4	15.2991	2.11	2.0640	145.64	2.95	18.87	12.50	8.93	12.26
	o-xylene	4	10.9938	0.74	1.0323	149.57	0.87	13.46	1.66	4.90	88.19
	p-xylene	4	8.9739	0.83	1.0964	149.51	0.86	6.18	8.17	3.28	75.33
	tetrabutyltin	4	19.2556	3.34	0.5544	150.12	1.13	13.75	16.40	19.86	150.45
	tetraethyltin	5	15.3481	9.45	0.7116	148.73	6.31	17.69	20.42	24.33	121.38
	tetramethyltin	4	14.3788	4.89	0.8621	147.09	1.35	36.01	19.45	28.37	90.42
	tetrapropyltin	4	16.9356	3.89	0.6115	149.11	1.10	8.07	16.00	19.02	132.61
	toluene	4	10.6104	2.56	0.9051	145.10	1.51	15.73	1.81	5.83	78.27
	xenon	4	13.3659	1.66	1.3238	145.23	1.84	42.84	20.04	44.22	45.81
propane	1-octene	8	8.2883	2.05	1.5602	57.26	1.91	9.91	7.32	26.64	14.87
	1-tetradecene	8	5.8133	2.09	1.3094	58.74	1.92	40.78	16.66	19.75	25.65
						Gas systems					
argon	ethane	9	5.3472	1.20	4.7507	7729.39	1.72	12.61	–	–	–
	hydrogen	5	−0.2416	5.44	23.0413	3938.78	2.29	72.01	–	–	–
	i-butane	8	9.0204	4.68	2.6722	5654.17	1.33	71.90	–	–	–
	methane	9	3.2619	3.06	7.7281	8889.20	1.49	22.49	–	–	–
	n-butane	8	8.2614	3.00	2.8191	6520.36	1.24	67.17	–	–	–
	neon	25	1.8476	1.71	10.3605	6724.28	5.46	35.22	–	–	–
	propane	9	6.5346	0.93	3.6775	7706.29	0.78	38.79	–	–	–
carbon dioxide	ethylene	48	7.7370	7.19	2.9026	-3.87	4.79	9.12	–	–	–
	hydrogen	7	1.5266	0.34	19.8027	5898.70	0.28	73.95	–	–	–
carbon monoxide	helium	7	-3.2255	0.51	22.1377	5018.43	0.16	69.03	–	–	–
	hydrogen	7	-0.4555	0.26	22.1377	5018.43	0.16	70.85	–	–	–
deuterium	hydrogen	5	-2.1082	6.76	34.7676	2840.99	1.14	35.80	–	–	–
ethane	nitrogen	14	5.9819	1.46	4.8313	6847.25	0.95	11.79	–	–	–
ethylene	carbon dioxide	49	5.9946	5.65	3.0975	5.29	3.53	9.95	–	–	–
	nitrogen	7	4.8917	0.69	5.0043	5395.35	0.38	8.64	–	–	–
helium	hydrogen	17	−3.7257	12.78	49.5883	5467.93	5.16	51.24	–	–	–
krypton	argon	6	6.9846	1.07	5.6514	11563.83	2.91	32.57	–	–	–
	helium	6	2.2108	0.93	22.0575	9617.38	2.38	81.76	–	–	–
	neon	17	6.7151	2.44	9.0618	8120.62	2.92	53.32	–	–	–
	xenon	8	10.6048	1.07	3.3325	13066.53	2.29	9.25	–	–	–
methane	carbon dioxide	10	6.9849	1.75	5.9479	6501.16	1.72	19.26	–	–	–
	tetrachloroethene	5	11.9925	0.74	2.8076	7640.69	0.11	110.69	–	–	–

Table 3 (*Continued*)

System		$D_{12,Real}$ (This work: Eqs. (8)–(17))			DHB (Eq. (27))			Zhu (Eqs. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Solvent (1)	Solute (2)	NDP	$E_D \times 10^9$ (erg/mol)	*AARD*	$B \times 10^7$ (mol/cm s$K^{1/2}$)	V_D (cm^3/mol)	*AARD*	*AARD*	*AARD*	*AARD*	*AARD*
neon	deuterium	5	0.4004	3.80	24.0282	3212.22	1.12	46.96	–	–	–
	helium	24	−0.9529	5.87	28.0397	2125.92	1.25	57.07	–	–	–
	hydrogen	5	−2.0151	6.68	31.7987	2881.11	0.63	61.10	–	–	–
	xenon	6	2.6328	0.96	6.4366	4241.29	0.78	61.51	–	–	–
nitrogen	helium	8	−0.8881	3.09	21.4938	6427.19	2.11	66.53	–	–	–
	hydrogen	29	−2.0425	1.53	23.3826	4968.86	1.25	72.28	–	–	–
	methane	7	3.2152	2.60	7.4175	6561.84	1.81	18.82	–	–	–
	n-butane	5	10.1662	7.23	2.6491	3362.34	0.96	75.74	–	–	–
	propane	6	9.7514	5.81	3.2798	4492.50	0.74	52.52	–	–	–
oxygen	helium	8	−1.1792	1.69	21.0509	4501.28	1.36	66.70	–	–	–
	hydrogen	13	−3.1834	2.65	26.2335	6132.89	0.50	72.82	–	–	–
sulfur hexafluoride	cyclohexane	5	10.4738	0.21	1.1504	8141.63	0.12	2.50	–	–	–
	methylcyclohexane	5	12.2512	0.88	1.1703	10547.92	0.32	11.66	–	–	–
tetrafluoromethane	1,1,1-trichloroethane	5	7.6343	0.80	1.4470	7233.94	0.86	37.93	–	–	–
	tetrachloroethene	5	9.6719	2.42	1.0459	3426.96	0.92	51.75	–	–	–

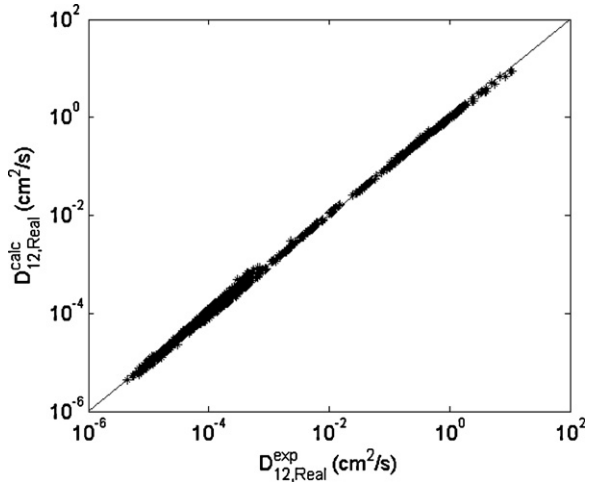

Fig. 3. Comparison between calculated and experimental tracer diffusivities for all systems studied in log-log scale.

vitamin K_3. In these cases, the unique properties already known were the molecular weight and boiling point. Note that most group contribution methods available to estimate T_c, P_c and V_c do not comprehend metallic atoms like Co, Fe, Pd, Cu, Sn. Hence, the critical constants have been calculated by Klincewicz [13,52]. Even so, the *AARD*s found were surprisingly small for these systems: 1.26 to 9.45%.

In Fig. 2 the calculated diffusivities for gas, liquid and supercritical systems are plotted against their experimental values. The three graphics show a good distribution along diagonal which confirms the new model does not exhibit systematic deviations. This fact, in conjunction with the low global *AARD*s of Table 4, evidences the potential of our model to represent tracer diffusivities of real molecules: *AARD*(Gas) = 3.78%, *AARD*(Liquid) = 5.35%, and *AARD*(SCF) = 4.32%. Hence, one parameter seems sufficient to reach excellent results for a huge number of systems over wide ranges of temperature and density. In order to emphasize the good performance of the new model over the global range of diffusion coefficients, particularly at low temperatures and high densities where D_{12} is small, a comparison between the calculated and the experimental values of all systems studied is shown in Fig. 3 in log-log scale. The thin and almost linear distribution along diagonal highlights the accurate model behaviour.

In Table 4 the global deviations found for the remaining models are listed: $AARD_{WC}$ = 16.47%, $AARD_{LR}$ = 26.54%, $AARD_{LT}$ = 36.04%, $AARD_{Zhu}$ = 37.66%, $AARD_{DHB}$ = 3.84%. Despite possessing no parameters, the errors offered by the former four equations are not acceptable, particularly those for Lusis-Ratcliff [3,41], Lai-Tan [42], and Zhu et al. [38]. On the other hand, the free volume equation of Dymond [1,2,39] correlates experimental data very well, which may be attributed in part to the two parameters embodied: B and V_D (see Eq. (27)). Nonetheless, its result is comparable to that accomplished by our 1-parameter equation: 3.84 *versus* 4.40%. It is worth to note that the DHB equation presented two physically meaningless results: quite different minimum diffusive free volumes (V_D) for the same solvent, which is incorrect, and even negative values (see Table 3). For instance, for CO_2 (solvent) the following V_D values have been fitted: −49.61, −34.23, −26.59 cm^3 mol^{-1}, etc. Moreover, the DHB equation should be used only for interpolation, which limits its application outside the fitting interval.

The prediction capability of our model has been also tested in this paper and compared with DHB performance according to the following procedure: (i) 118 systems containing experimental data at distinct temperatures have been chosen in order to fit E_D (new model), and B and V_D (DHB model) to the highest temperature

Table 4
Relative deviations for the supercritical, liquid and gas systems.

Type of system	NDP	NS	$D_{12,Real}$ (Eqs. (8)–(17))	DHB (Eq. (27))	Zhu. (Eq. (21)–(26))	WC (Eq. (18))	LR (Eq. (19))	LT (Eq. (20))
Supercritical	4324	173	4.32	3.77	36.98	13.76	24.88	27.28
Liquid	675	104	5.35	5.27	40.53	33.85	37.16	92.15
Gas	422	37	3.78	2.33	39.95	–	–	–
Global	5421	314	4.40	3.84	37.66	16.47	26.54	36.04

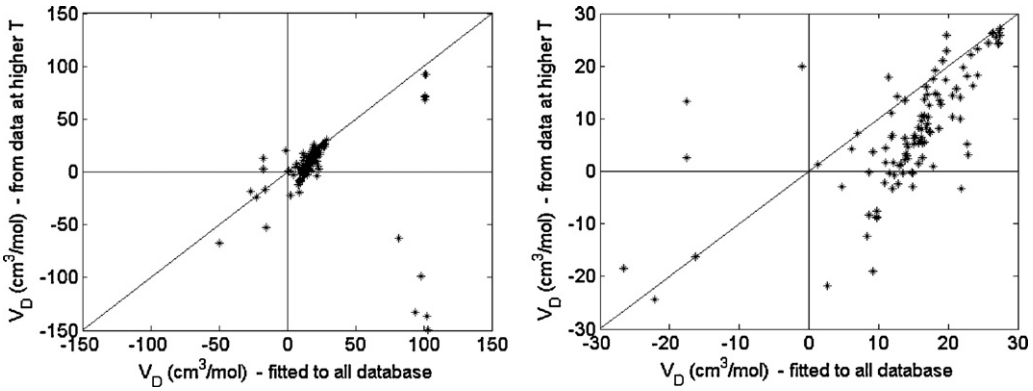

Fig. 4. V_D parameter of DHB model (Eq. (27)) regressed using all database *versus* V_D fitted to data at only the highest temperature. Note the different scale of the two graphs (118 systems studied totalizing 3665 experimental points).

Table 5
Average absolute relative deviations calculated for: (i) correlation of the complete database (the same global values of Table 4; (ii) estimation of the diffusivities using parameters fitted only to the set of data at highest temperatures. Comparison accomplished for 118 systems/3665 points.

Model	*AARD* (all data fitted)	*AARD* (partial fitting)
DHB	3.84	15.74
New model	4.40	5.27

data; (ii) The parameters so obtained were subsequently used to estimate the tracer diffusivities by the new model and by DHB equation for the remaining lower temperatures. The results evidenced that the DHB prediction capacity is questionable since its *AARD* for prediction is 15.74%, whereas our new model only rises up to 5.27%. (Remember that the initially calculated deviations for complete correlation were 3.84 and 4.40%, respectively—see Table 4). Table 5 summarises this comparison. Furthermore, the V_D values fitted to all data and to part of them vary too much, as Fig. 4 points out. Inclusively, some V_D values jump from positive to negative and vice-versa. In contrast, our E_D values remain approximately the same as Fig. 5 illustrates.

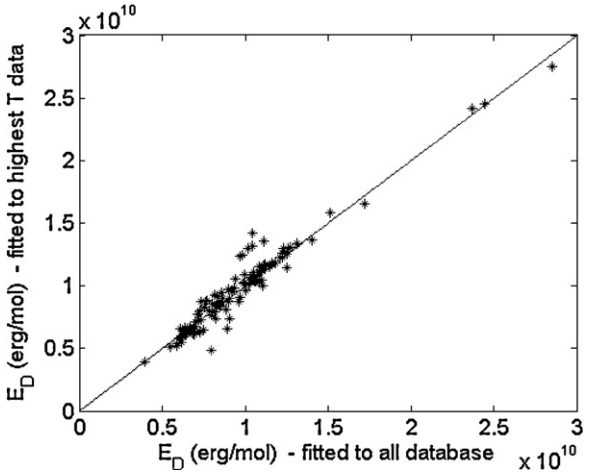

Fig. 5. E_D parameter of our new model regressed using all database *versus* E_D fitted to data at only the highest temperature (118 systems studied totalizing 3665 experimental points).

6. Conclusions

In this work a new model for tracer diffusion coefficients of real systems is proposed. It was derived on the basis of the HS model fluid, following a systematic derivation whereby the softness of repulsive interactions and the contribution of attractive forces were taken into account by means of the effective hard sphere diameter method and by coupling an Arrhenius exponential term. The model is explicit and straightforward: the diffusion coefficient is computed as function of temperature and density, and calls a diffusive parameter E_D, i.e. $D_{12,Real} = D_{12,Real}(T, \rho_1; E_D)$. This parameter can be obtained by linear optimization. The validation of the model has been accomplished with the largest data base ever compiled up till now, composed of 314 binary systems and 5421 experimental tracer diffusivities. All properties for the 205 molecules involved were collected and presented here. The new model provides very good results for gas, liquid and supercritical systems over wide ranges of temperature and density, giving rise to a global average absolute relative deviation of only 4.40%. It also offers excellent representations for systems whose critical constants necessary for the calculation of LJ energy and diameter had to be estimated previously. Finally it must be emphasized its good prediction capability.

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