On predicting self-diffusion coefficients in fluids

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Abstract

A modification of an existing correlative equation for self-diffusion coefficients is presented. A free-volume theory for liquids has been corrected to reproduce diffusivities of hard-sphere and Lennard-Jones fluids from low-density limit to melting points, and has been applied to correlate a wide database of nonpolar, polar, quantic and hydrogen-bonding substances, although it is unable to fit helium, water and hydrogen fluoride. The adjustable parameters are generalized with available fluid properties, and the three resulting predictive formulas present lower deviations than other correlative equations used in a predictive way for non-quantic and non-associated fluids.

Keywords: Diffusion, Dynamic simulation, Hard-sphere, Lennard-Jones, Mathematical modelling, Theory of liquids.

1. Introduction

The abundance of experimental self-diffusivities in liquids, gases and vapours in the last century, and the molecular dynamics simulations for simple fluids have generated many empirical or semiempirical formulas for dense fluids. The models of Ruckenstein and Liu, [1] Liu et al. [2] and Dariva et al. [3,4] can be considered the most significant proposed between 1990 and 2000, because of their general validity (applicable over wide ranges of temperature and pressure for non hydrogen-bonded compounds) and the posibility of using them to estimate binary diffusion coefficients of solutes at infinite dilution (Liu and Ruckenstein, [5] Liu et al. [6], Dariva et al. [3,4]), which are needed in the modelling and design of mass transfer operations. The three are good for correlating experimental data, but their predictive power is limited. Recently, Zhu et al. [7] and Zabaloy et al. [8] have proposed purely predictive expressions for self-diffusion, although their average absolute deviation (AAD) are high (18.51% for 1226 points of 17 substances in the case of Zhu and 16.27% for 1043 points of 20 substances in the case of Zabaloy). The theoretical background of the five equations is the same: describing the potential energy of the molecules (attractive forces+repulsive forces) with the Lennard-Jones potential (LJ).

Far from these models, generalized charts such as those of Slattery and Bird [9], Tee et al. [10], Ramanan and Hamrin [11] and Takahashi [12] were the first attempts to deal with dense gases and liquids, but were all based on very little experimental data. Only the empirical equations of Lee and Thodos [13] compiled enough data to compare their results with those of LJ expressions.

In the present work, the free volume model of Boned et al. [14] has been corrected to reproduce the low-density limit using the hard-sphere scheme, and the global formula is able to correlate LJ fluids. Boned and coworkers developed mathematical expressions for viscosity and self-diffusion in liquids, so the adjustable parameters could be fitted at the same time, obtaining a diffusivity-viscosity relation similar to that obtained by Dullien [15] and Vadovic and Colver [16]. The viscosity formula was applicable to gases, but the diffusion equation was not. Both were functions of temperature, pressure and density, which is very interesting because of the pressure dependence: liquid densities do not greatly vary with pressure, but self-diffusion and viscosity do, and so functions of temperature and density alone are highly sensitive to errors in estimations of compressed liquid density values, but if the pressure dependence is added the sensitivity could be reduced.

Surely, the common correlative parameters in the equations of diffusion and viscosity will not have the same numerical values, although they represent the same concepts, because it has been proven that the Dullien relation is not rigurously valid [17, 18]. So, only self-diffusion data from the literature were compiled, and the parameters obtained were generalized in three ways: with properties of each compound such as molar mass, critical temperatures and volumes, acentricities and number of atoms; with the Corresponding Sates Principle (CSP) like Xiang [19] and with the descriptors of the Linear Solvation Energy Relationship (LSER) like Mutelet and Rogalski [20]. The correlative power is good for quantic and hydrogen-bonding substances, excluding helium, water, hydrogen fluoride and pentanol isomers, but the predictive formulas are unable to reproduce any of the two cases.

2. Mathematical modelling

2.1. The original free-volume model

The free volume model is a theory of liquids stipulating that diffusion takes places because there exist holes between the molecules, and the continuous motion of molecules causes a variation in the size of these holes. A molecule undergoes a diffusive movement when a void of at least a minimum size of $V^{\min}$ is formed adjacent to it [21].

Boned et al. [14] extended to self-diffusion coefficients the viscosity model of Allal et al. [22], which treated viscosity as the sum of the low-density limit η^0, and a high-density term η_f. This assumption was not new. As Allal et al. clearly indicated in their paper, other authors considered it with the aim of representing simultaneously dense and gaseous fluid states and the transition between them. The originality was in selecting for η_f the following mathematical expression, due to Bueche [23]:

$$\eta_\mathrm{f} = \rho\xi\langle r\rangle^2 \tag{1}$$

where ρ is the number density, ξ the friction coefficient and $\langle r\rangle^2$ a characteristic molecular dimension (not exactly the square of the radius). The self-diffusivity D can be obtained from the friction coefficient, the absolute temperature (T) and the Boltzmann constant (k) with the Nernst-Einstein equation

$$D=kT/\xi \tag{2}$$

and the free-volume theory was employed to obtain an expression for ξ,

$$\xi = \frac{U}{l_\mathrm{f}}\sqrt{\frac{m}{3kT}}\exp\left\{\gamma\frac{V^{\min}}{V^{\mathrm{free}}}\right\} \tag{3}$$

U is the interaction potential energy between molecules ($U=C_1\rho+P/\rho$, being P the absolute pressure), and this energy dissipates through the characteristic length l_f due to friction. The numerical factor γ takes into account the overlapping of free volumes, V^{min} is roughly the molecular volume, m the molecular mass and V^{free} the free volume, usually defined as the difference between the molar volume and the molecular volume [24, 25]. Nevertheless, Allal et al. did not use this definition, but another that employed the interaction potential energy, U

$$V^{\mathrm{free}} \propto V\left(\frac{2kT}{U}\right)^{3/2} \tag{4}$$

so, the self-diffusion is written as

$$D = \frac{l_{\mathrm{f}} kT}{C_1\rho + P/\rho}\sqrt{\frac{3kT}{m}}\exp\left[-\gamma^*\left(\frac{C_1\rho + P/\rho}{kT}\right)^{3/2}\right] \tag{5}$$

and the three fitting parameters are γ^*, C_1 and l_{f}.

2.2. Corrections to the model of Boned et al.

It can be seen that Eq. (5) does not reproduce the Chapman-Enskog expression in the low-density limit [26, 27].

$$D^0 = \frac{3}{8\rho\,\sigma^2}\sqrt{\frac{kT}{\pi m}}\frac{1}{\Omega_{\mathrm{D}}} \tag{6}$$

where σ is the molecular diameter and Ω_{D} a collision integral, which is a function of the molecular reduced temperature, $T^* = kT/\varepsilon$. In a previous paper, we have reviewed the Enskog theory (E), the hard-sphere model (HS) and the Lennard-Jones fluids (LJ), and their application to self-diffusivities [28]. Inspired by the empirical formula of Hippler et al., described there, we propose the following correction to the formula of Boned et al.:

$$D = \frac{\sqrt{\dfrac{3kT}{m}}\, l_{\mathrm{f}} \left(\dfrac{\mathrm{C}_1 \rho}{kT} + \dfrac{P}{\rho kT} \right)^{-1} \exp\left[-\gamma * \left(\dfrac{\mathrm{C}_1 \rho}{kT} + \dfrac{P}{\rho kT} \right)^{3/2} \right]}{1 - \exp\left\{ -\dfrac{8}{3} \sqrt{3\pi}\, \rho \sigma^2 l_{\mathrm{f}} \exp(-\gamma *) \Omega_{\mathrm{D}} f^{\,\mathrm{corr}} \right\}} \tag{7}$$

The unknown function $f^{\,\mathrm{corr}}$ will be determined from molecular simulations of LJ and HS fluids. The molecular reduced self-diffusivity can be expressed as

$$D* = \frac{D}{\sigma} \left(\frac{m}{\varepsilon} \right)^{1/2} = \frac{l_{\mathrm{f}} * \sqrt{3T *} \left(\mathrm{C}_1 * \dfrac{\rho *}{T *} + Z \right)^{-1} \exp\left[-\gamma * \left(\mathrm{C}_1 * \dfrac{\rho *}{T *} + Z \right)^{3/2} \right]}{1 - \exp\left\{ -\dfrac{8}{3} \sqrt{3\pi}\, \rho * l_{\mathrm{f}} * \exp(-\gamma *) \Omega_{\mathrm{D}} f^{\,\mathrm{corr}} \right\}} \tag{8}$$

where Z is the compressibility factor, $\rho *=\rho \sigma^3$, $l_{\mathrm{f}} * = l_{\mathrm{f}} / \sigma$ and $\mathrm{C}_1 *=k\mathrm{C}_1/(\varepsilon \sigma^3)$. To transform Eq. (8) into an HS equation, it could be logical to invert the two steps carried out by Chandler [29]:

- Transforming effective densities into normal densities, but this model has no effective diameters.
- Rejecting the terms that represent the rotational-translational coupling parameter or attractive forces. Such rejection can be made if $T* \to +\infty$, as inferred from the literature [30, 5, 6]

$$\frac{D^{\mathrm{HS}}}{D^{E}} = \frac{\frac{8}{3}\sqrt{3\pi}\rho * l_f *}{1 - exp\left\{-\frac{8}{3}\sqrt{3\pi}\rho * l_f * exp(-\gamma *) f^{\mathrm{corr}}\right\}} \text{ x } \frac{g(\sigma)\, exp\left[-\gamma * \left(Z^{\mathrm{HS}}\right)^{1.5}\right]}{Z^{\mathrm{HS}}} \tag{9}$$

$g(\sigma)$ is the radial distribution upon contact [31, 32] and Z^{HS} is obtained from it. Eq.(9) is compared with the molecular simulations of Heyes et al. [31] in Fig.1: the original model of Boned et al. can correlate data for $\rho^*> 0.45$ fitting only l_f^* and γ^*. If the same parameters are taken, and $f^{corr} =1.0$, the high-density region is well-represented, but at low and middle densities the diffusivities are overpredicted. The best performance of Eq. (9) is obtained when

$$f^{corr} = (Z^{HS})^{0.6} \tag{10}$$

In Fig.1 the molecular simulation of Woodcock and Angell is also represented [33]. It was carried out in a metastable fluid, at densities greater than that of the liquid-solid transition, so, our model not necessarily has to follow its trend.

Table 1 compiles the values of l_f^*, γ^* and of the Average Absolute Deviation (AAD) of fitting data of Heyes et al. and of other sources [34-37]. The results are very good.

Now, Eqs. (8) and (10) would be able to correlate diffusion in LJ systems, but we have empirically modified f^{corr} for incorporating the temperature dependence that the HS model obviates.

$$f^{corr} = 1 + \frac{Z^{0.6} - 1}{1 + \exp\{-6(T^* - 1.33)\}} \tag{11}$$

The simulation data of Kataoka and Fujita [38], Rowley and Painter [39] and Meier et al. [40], which cover all fluid states, have been chosen to check the ability of Eqs. (8) and (11). As the three groups of authors only provide ρ^*-D^*-T^* tables, figures or formulas, the compressibility factor has been calculated from the pressures obtained by Meier in his Thesis [41]. Moreover, some data are placed in thermodynamic metastable liquid-vapour biphasic zone, so they have been rejected when saturated liquid and vapour densities [42] and vapour pressures [43] were known. The results are shown in Table 2 and in Figs. 2, 3, and 4. It has to be pointed out that the collision integral values computed by Kataoka and Fujita are higher than those commonly accepted [26], and that none of the models mentioned above in Section 1 can reproduce the maxima and minima of ρ^*D^*, except the formula of Zabaloy et al.

3. Existing models

3.1. Equation of Ruckenstein and Liu [1]

$$D = \frac{A_{\mathrm{D}} kT}{\frac{8}{3}\rho(\sigma^{\mathrm{eff}})^2 (\pi mkT)^{1/2} \left[g(\sigma)\frac{D^{\mathrm{E}}}{D^{\mathrm{HS}}} + \frac{0.4}{(T^*)^{1.5}} \right]} \tag{12}$$

$$\sigma^{\mathrm{eff}} = 1.1532\sigma^{\mathrm{LJ}} \left[1 + \left(\frac{T^*}{0.527} \right)^{1/2} \right]^{-1/6} \tag{13}$$

$$\frac{D^{\mathrm{HS}}}{D^{\mathrm{E}}} = 1 + 0.94605(\rho^*)^{1.5} + 1.4022(\rho^*)^3 - 5.6898(\rho^*)^5 + 2.6626(\rho^*)^7 \tag{14}$$

$$\rho^* = \rho(\sigma^{\mathrm{eff}})^3 \tag{15}$$

$\varepsilon^{\mathrm{LJ}}$, σ^{LJ} and A_{D} can be correlated with the the critical temperature (T_{c}), the critical volume (V_{c}) and the Pitzer's acentric factor (ω) using

$$\frac{\varepsilon^{\mathrm{LJ}}}{k} = \frac{T_{\mathrm{c}}}{1.2593} \tag{16}$$

$$\sigma^{\mathrm{LJ}} = (0.7889 V_{\mathrm{c}}^{1/3}) \times 10^{-8} \tag{17}$$

$$A_{\mathrm{D}} = 0.9673 - 0.2527\omega - 0.7\omega^2 \tag{18}$$

For methane and noble gases, A_{D} =1.0

3.2. Equation of Liu et al. [2]

$$D = \frac{kT}{\frac{8}{3}\rho(\sigma^{\mathrm{eff}})^2(\pi mkT)^{1/2}} \exp\left[-\frac{0.75\rho*}{1.2588-\rho*} - \frac{0.27862}{T*}\right] \tag{19}$$

$$\rho* = \rho(\sigma^{\mathrm{eff}})^3 \tag{20}$$

$$\sigma^{\mathrm{eff}} = 2^{1/6}\sigma^{\mathrm{LJ}}\left[1+(1.3229T*)^{1/2}\right]^{-1/6} \tag{21}$$

σ^{LJ} and ε^{LJ} were the two fitting parameters, and could be roughly calculated with the critical pressure and temperature by

$$\frac{\varepsilon^{\mathrm{LJ}}}{k} = 0.774T_{\mathrm{c}} \tag{22}$$

$$\sigma^{\mathrm{LJ}} = 10^{-10}\left[0.17791 + 11.779\times10^5\frac{T_{\mathrm{c}}}{P_{\mathrm{c}}} - 0.049029\times10^{10}\left(\frac{T_{\mathrm{c}}}{P_{\mathrm{c}}}\right)^2\right]^{1/3} \tag{23}$$

3.3. Equation of Dariva et al. [3]

$$D = \frac{kT}{\frac{8}{3}\rho(\sigma^{\mathrm{eff}})^2(\pi mkT)^{1/2}}\left(1-\frac{\rho*}{1.09}\right)\left[1+0.4(\rho*)^2 - 0.83(\rho*)^4\right] \tag{24}$$

$$\rho* = \rho(\sigma^{\mathrm{eff}})^3 \tag{25}$$

$$\sigma^{\mathrm{eff}} = 2^{1/6}\sigma^{\mathrm{LJ}}\left\{1+\left[\frac{T*-0.03367(T*)^2+0.0003935(T*)^4}{1.5001(1-0.09835\rho*+0.04937(\rho*)^2-0.1415(\rho*)^3)}\right]\right\}^{-1/6} \tag{26}$$

The adjustable parameter is σ^{LJ}. Although these authors do not correlate this with critical volume, we have obtained

$$\sigma^{\mathrm{LJ}} = (0.7884 V_{\mathrm{c}}^{1/3}) \times 10^{-8} \tag{27}$$

and the energy parameter is related with the critical temperature by [4]

$$\frac{\varepsilon^{\mathrm{LJ}}}{k} = 0.77 T_{\mathrm{c}} \tag{28}$$

3.4. Equation of Zhu et al.[7]

Zhu and coworkers adjusted the molecular simulation data of Rowley and Painter [39] for LJ fluids and defined effective energy and size parameters which include $\rho_{\mathrm{r}}=\rho/\rho_{\mathrm{c}}$ and $T_{\mathrm{r}}=T/T_{\mathrm{c}}$.

$$D = \frac{kT}{\frac{8}{3}\rho(\sigma^{\mathrm{eff}})^2(\pi m k T)^{1/2}}\left(1 - \frac{\rho\ \ *}{1.029079(T*)^{0.165377}}\right) \times exp\left(-\frac{\rho*}{2T*}\right)$$
$$\times\left[1 + (\rho\ *)^{0.126978}\left(\frac{0.596103(\rho*-1)}{0.539292(\rho*-1)+(T*)^{(0.400152-0.41054\rho*)}} + 0.68856\right)\right]$$

(29)

$$\frac{\varepsilon^{\mathrm{eff}}}{k} = \frac{\varepsilon^{\mathrm{LJ}}}{k}\left[1 + 0.47527332\rho_{\mathrm{r}} + (0.06300484 + 0.12374707\rho_{\mathrm{r}})T_{\mathrm{r}}\right] \tag{30}$$

$$\frac{\varepsilon^{\mathrm{LJ}}}{k} = \frac{T_{\mathrm{c}}}{1.313} \tag{31}$$

$$\sigma^{\mathrm{eff}} = \sigma^{\mathrm{LJ}}\left[1 - 0.0368868\rho_{\mathrm{r}} + (0.00006945 + 0.01089228\rho_{\mathrm{r}})T_{\mathrm{r}}\right] \qquad (32)$$

$$\sigma^{\mathrm{LJ}} = (0.8014V_{\mathrm{c}}^{1/3}) \times 10^{-8} \qquad (33)$$

$$\rho^* = \rho(\sigma^{\mathrm{eff}})^3 \qquad (34)$$

$$T^* = \frac{T}{(\varepsilon^{\mathrm{eff}}/k)} \qquad (35)$$

3.5. Equation of Zabaloy et al [8]

They adjusted the molecular simulation of Meier et al. [40] to the polynomial expression:

$$\rho^* D^* = (\rho^* D^*)^0 + \sum_{\mathrm{i}=1}^{4}\sum_{\mathrm{j}=1}^{6} b_{\mathrm{ji}} \frac{(\rho^*)^{\mathrm{i}}}{(T^*)^{(\mathrm{j}-1)}} \qquad (36)$$

where the coefficients b_{ji} are empirical, and the density is obtained through the equation of state of Kolafa and Nezbeda [44]. This formula is only valid when reduced density is smaller than $\rho^*=0.92146891\ (T^*)^{0.21839684}$ and $0.7 \le T^* \le 6$.

$$\varepsilon^{\mathrm{LJ}} = \frac{kT_{\mathrm{c}}}{1.3396} \qquad (37)$$

$$\sigma^{\mathrm{LJ}} = \left(\frac{kT_{\mathrm{c}}}{P_{\mathrm{c}}}\frac{0.1405}{1.3396}\right)^{1/3} \qquad (38)$$

3.6. Correlation of Lee and Thodos. [13]

This is based on the empirical analysis of a great deal of experimental data, and is divided in two parts: when $\frac{\rho_\mathrm{r}}{T_\mathrm{r}^{0.1}} \leq 1.00$

$$D\left(\frac{M^{1/2}}{P_\mathrm{c}^{1/2}V_\mathrm{c}^{5/6}}\right) = 7.646\times10^{-9}\frac{T_\mathrm{r}}{\rho_\mathrm{r}} \tag{39.a}$$

If $\frac{\rho_\mathrm{r}}{T_\mathrm{r}^{0.1}} > 1.00$

$$D\left(\frac{M^{1/2}}{P_\mathrm{c}^{1/2}V_\mathrm{c}^{5/6}}\right) = 9.93\times10^{-9}T_\mathrm{r}\left[0.7094\left(\frac{\left(\frac{\rho_\mathrm{r}}{T_\mathrm{r}^{0.1}}\right)_\mathrm{t} - \left(\frac{\rho_\mathrm{r}}{T_\mathrm{r}^{0.1}}\right)}{\left(\frac{\rho_r}{T_\mathrm{r}^{0.1}}\right)_\mathrm{t} - 1}\right) + 0.1916\right]^{2.5} \tag{39.b}$$

The subscript ‘t’ represents triple point: temperature and density are reduced to temperature and solid density in that point. As the solid density is usually unknown, it can be treated as the fitting parameter, or calculated as

$$\left(\frac{1}{\rho_\mathrm{r}}\right)_\mathrm{t} = 1.21\left(\frac{2Z_\mathrm{c} - 1 + \sqrt{4Z_\mathrm{c}^2 + 1}}{2Z_\mathrm{c} + 1 + \sqrt{4Z_\mathrm{c}^2 + 1}}\right) \tag{40}$$

Nevertheless, Lee and Thodos indicate that Eq. (39.b) is very sensitive to the solid density values, so considerable errors can be obtained if Eq. (40) is used to predict them. At high reduced temperatures, Eq. (39.a) deviates from Eq. (6) because it is based on the experimental data of Ember et al. [45] and Pakurar and Ferron [46] for carbon dioxide. According to these authors, LJ potential can not describe well this linear molecule (as Galliero et al. have recently pointed out [47]), and it is not possible to employ the same values of σ^{LJ} and ε^{LJ} for all transport properties. Moreover, Ember, Pakurar and Ferron hypothetized that LJ potential fails at high temperatures for non-spherical molecules. However, in this work these data have been rejected because they were questioned in terms of complex molecular dynamics calculations [48], and other experimental points at high reduced temperatures are very scarce, being only available for hydrogen [49], neon [50] and krypton [51], which can be treated as LJ fluids without any problem.

4. Application to real fluids.

A supplementary Table A1 shows the compiled data, together with the thermodynamic states in which the self-diffusion coefficients are available and bibliographic references. The substances have been selected because densities, critical points and other properties were available (or calculable). These properties, together with some comments can be seen in a supplementary Table A2.

In addition we highlight that

- Methane data of Jeffries and Drickamer [52] are considered erroneous, following the considerations of Thodos and coworkers [53, 54].
- For ethane, the experimental results of Wade and Waugh [55] have been rejected, because of the discrepancy with the data of Gaven et al. [56] and Greiner-Schmidt et al. [57]
- For 2,2-dimethylbutane there exist important discrepancies between Polzin and Weiss [58] and Bachl et al. [30] except at low temperatures. The data of McCall et al. [59] are intermediate, but the pressure is too low to deduce which are the correct ones. Otherwise, in the work of Bachl et al. [30] only *D vs.* ρ data are given, and a good

comparison at low temperatures is difficult (slight errors in density become great errors in the estimation of pressure). We only take the experimental points of McCall et al. [59]

- The experimental error in acetylene points of Mueller and Cahill [60] is suspected to be high.
- For cyclohexane, according to Freer and Sherwood [61] we have rejected the self-diffusivities of Hawlicka and Reimschüssel [62]. As 2,2-dimethylbutane, there exist large differences between the two sources: Jonas et al. [63] and Polzin and Weiss [58] above 358 K, and we have not taken the high temperature points of either because the other references do not permit us to know the correct data.
- In nitromethane [64-68] and nitrobenzene [62, 66] the experimental points of several authors follows two different tendencies.
- For liquid tetramethylsilane, there exist significant differences between Douglass et al. [69] and Kessler et al. [70] along the saturation line (or atmospheric pressure), but there is no way of determining which are the correct ones. Only the self-diffusivities at elevated pressures of Douglass et al. [69] have been taken because of the good concordance with Parkhust and Jonas [71].
- Along the saturation line the self-diffusivities of several authors coincide at low temperatures, but differ when this variable rises. This is the case of chlorobenzene [17, 66], *n*-pentane [69, 70], dichloromethane [72-74] and hexafluorobenzene [75, 76].
- From McCall et al. [64] we have only selected data of cyclohexane at 298.16 K (between 0.1 and 33.1 MPa) and acetone at 0.1 MPa in the range 182.86 - 301.16 K, and 0.1-50 MPa at 301.16 K after comparison with other literature values. The correlative equations given by these authors have no application range and the self-diffusivities of benzene were rejected by Falcone et al. [77]

- All experimental data of Kitchlew and Nageswara Rao [78] have been rejected, according to Ertl [79]. Benzene, chlorobenzene, pyridine and nitrobenzene differ greatly compared with other sources.
- O´Reilly et al. [80] states that the critical temperature of *tert*-buthyl chloride is 490 K, which is in opposition to the value of 507 K given by other sources (Reid et al. [27], Lide [81], HYSYS database and Korea thermophysical properties Data Bank). However, the data measured by these researchers beyond 490K are clearly supercritical diffusivities, so only data at low temperatures have been taken.
- For the 1,2-dibromotetrafluoroethane of Polzin and Weiss [58] the experimental points have been read from the article, graph since there is an error in the correlative formula provided by the authors. In the same article, there exist errors in the equations for calculating densities, detected thanks to the articles of Cibulka and Takagi [82, 83].
- For argon the value of Cini-Castagnoli and Ricci [84] has been removed because of the discrepancy with Corbett and Wang [85] and McLaughlin [86].
- The xenon results of Yen and Norberg [87] are lower than the data of other authors, and have also been removed.
- The carbon dioxide of Robb and Drickamer [88] is considered erroneous [89].
- Woolf [90] considered that the self-diffusivities of carbon disulfide obtained by Koeller and Drickamer [91] are erroneous because of failures in their experimental method.
- Hartland and Lipsicas [92] do not specify the pressure of their low-density data of hydrogen, but as they stated that the product ρD is constant for densities lower than 40.47 kg m^{-3}, atmospheric pressure has been supposed. Only in hydrogen have the corrections due to the use of isotopes for experimental measures have been taken into account, because the diffusion of D_2 in H_2 at low density is 15.5% lower than hydrogen self-diffusion [49].

- For water, self-diffusion coefficients at low temperatures of Harris and Woolf [93] surely are the correct ones, becuse of their coincidence with Polzin and Weiss [58] and tracer diffusivities of THO in H_2O [94], DTO in D_2O [95] and self-diffusion of D_2O [96, 97]. All experimental points of Kiselnik et al. [98] and those of Krinicky et al. [99] near 273.15 K have been rejected.
- Lamb et al. [100] suspect that there are errors in the D_2O diffusivities of Wilbur et al. [96] because of inconsistencies in the Stokes-Einstein formula, but they do not quantify these errors.
- The saturated liquid HF of Karger et al. [101] is placed between the two data sets of O'Reilly [102, 103].

The vapour pressures have been taken from the NIST website (http://webbook.nist.gov/chemistry/fluid/) and from the “Korea Thermophysical Properties Data Bank” (http://www.cheric.org/kdb/) . If these were not available, we have taken them from HYSYS data bank or from the handbook of Perry and Green [104].

Boned et al. [14] proposed a way of calculating the three fitting parameters in liquids by linear regression. This was based on the representation of

$$-ln\left[\frac{D*}{\sqrt{3T*}}\left(C_1 * \frac{\rho*}{T*} + Z\right)\right] \quad \text{vs.} \quad \left(C_1 * \frac{\rho*}{T*} + Z\right)^{3/2} \tag{41}$$

and C_1* was varied until a straight line was obtained. The slope of such a line was γ*, and the value in the origin was -$ln(l_f*)$. It can be proven that if experimental data only cover a narrow range of temperatures and pressures, or are measured at saturation, the calculation of the adjustable parameters is not possible, because a straight line is obtained with any value of C_1*.

Thus, the pressure dependence of the self-diffusion coefficient is determined by the constant C_1*.

The real substances have been treated as LJ fluids. The mathematical form of the collision integral proposed by Neufeld was selected [27, 28] and values of σ^{LJ} and ε^{LJ} have been calculated with Chung's formulas [27], except for hydrogen and deuterium, in which σ=2.959×10^{-10} m and ε/k=36.7 K were taken. These values come from the second virial coefficient [26] and reproduce the compiled low-density gaseous data [105] without quantum corrections in Ω_D.

The values of $ln(l_f*)$, γ* and C_1* are given in Table 3. They were determined by the least squares regression method, minimizing the following objective function (OF):

$$\mathrm{OF} = \sum_{i=1}^{\mathrm{NDP}} \left(1 - \frac{D_{\mathrm{i}}^{\mathrm{calc}}}{D_{\mathrm{i}}^{\mathrm{exp}}}\right)^2 \tag{42}$$

The average absolute deviation is defined as

$$\mathrm{AAD} = \frac{100}{\mathrm{NDP}} \sum_{i=1}^{\mathrm{NDP}} \left| \frac{D_{\mathrm{i}}^{\mathrm{calc}} - D_{\mathrm{i}}^{\mathrm{exp}}}{D_{\mathrm{i}}^{\mathrm{exp}}} \right| \tag{43}$$

where NDP is the number of data points of each substance and superscripts “calc” and “exp” mean “calculated” and “experimental”, respectively. Eqs. (8) and (11) can not be applied to He^3 nor H_2O due to their anomalies. Nevertheless, can neither these fitting parameters correlate the HF (even in the method of Boned and coworkers there are no values of C_1* that make a good linearization) and the AAD of 2-pentanol and 3-pentanol are very high. It has been pointed out that in these alcohols, the spatial position of hydroxil groups improves the hydrogen-bonding structures [106]. The same occurs in fluoroethanols, where 2,2-difluoroethanol forms more stable hydrogen bonds than 2-fluoroethanol or 2,2,2-trifluoroethanol [107], and this phenomenom justifies why its AAD is the highest of the three. For *N*-methylamine [108] and *N*-methylformamide [109] the hydrogen-bond strength is lower than in alcohols, and it could be thought that the present model fails in substances with strong hydrogen bonds. However, Yu and Gao [110] developed a correlative expression for self-diffusion in associated compounds and the fitting parameters reveal that hydrogen-bond strength is lower in HF than in alcohols.

Returning to Table 3, it has been shown that C_1* is the easiest generalizable parameter, with an AAD of 11.4% rejecting the associated substances

$$C_1 *= exp\Big\{-0.942552 - \frac{1.758548\times10^{-3}}{M} + 0.1165388 ln(T_c) + \\ + \frac{16.572630}{T_c} + 0.5208108 ln(10^6 V_c) + \frac{26.5997\times10^{-6}}{V_c} + 0.3414968\omega\Big\} \quad (44)$$

where *M* is the molar mass. Now there are two adjustable parameters, and saturated liquids can be correlated. The values are presented in Table 3 as well, and a global generalization of them would be

$$ln(l_f *) = -2.118586 - 0.2842494 ln(10^3 M) + 0.3644501 ln(T_c) + \\ 0.1607659 ln(10^6 V_c) \quad (45)$$

$$\gamma *= 0.01\, exp\Big\{ 2.106746 - 0.290965 ln(10^6 V_c) - 2.938654 \frac{\omega}{1+0.45\omega} -$$

$$-0.0157041 ln(10^6 V_c)\frac{\omega}{1+0.45\omega}+\frac{5.152255}{N_{\mathrm{atom}}}-1.305418\frac{ln(10^6 V_c)}{N_{\mathrm{atom}}}\Bigg\} \tag{46}$$

being N_{atom} the number of atoms in the molecule.

Several simple forms of the CSP have also been studied [19, 111]. Although strictly speaking, the LJ model follows a two-parameter CSP, σ^{LJ} and $\varepsilon^{\mathrm{LJ}}$ are fitting parameters, and they are not readily available as acentric factors, dipolar moments, radii of gyration or critical compressibilities. The best found includes the acentric factor and the radius of gyration (r_{g})

$$\mathrm{C}_1{*} = \exp\{2.147013 + 0.599979\omega + 0.1743645 r_{\mathrm{g}}\} \tag{47}$$

$$ln(l_f\ {*}) = -0.4141786 + 0.6937579\omega + 0.03885936 r_g \tag{48}$$

$$\gamma{*} = 0.01\exp\{0.5814897 - 1.124675\omega - 0.1901 r_{\mathrm{g}}\} \tag{49}$$

The AAD of this four-parameter CSP formula is shown in Table 4, and together with Eqs. (12),(19),(24),(29), (36) and (39), are all used in a predictive way. The overall AAD is not the arithmetic mean of the deviations of the substances, but the weighted average (employing the NDP for the weighting).

In this table a seven-parameter CSP with the LSER descriptors is also presented.

$$\begin{aligned}C_1\ {*}= exp\{\ 2.432771 + 0.195598 logL^{16} - 0.2188628 \mathit{\Delta} R - \\ -0.05093769\pi^{*} - 0.0292692\alpha^{\mathrm{H}} + 0.04416817\beta^{\mathrm{H}}\}\end{aligned} \tag{50}$$

$$ln(l_f\ {*}) = \text{-}0.2942431 + 0.1090247 logL^{16} - 0.05295435 \mathit{\Delta} R +$$

$$+0.06694504\pi^{*}+0.2297028\alpha^{\mathrm{H}}+0.3363918\beta^{\mathrm{H}} \quad (51)$$

$$\gamma *= 0.01\, exp\{\, 0.3828597 - 0.2840186 logL^{16} + 0.4459789\Delta R -$$
$$-0.06191012\pi^{*}-0.2055302\alpha^{\mathrm{H}}+0.1412839\beta^{\mathrm{H}}\} \quad (52)$$

L^{16} is the hexadecane-air partition coefficient, ΔR is the excess index of refraction, π^* is the dipolarity/polarizability, α^{H} is the total hydrogen-bond acidity and β^{H} is the total hydrogen-bond basicity. Although the LSER descriptors are first used to correlate partition coefficients [112], chromatographic retention volumes [113], activity coefficients at infinite dilution [114] and solubilities [115] and are temperature and pressure dependent [115-121], they were treated as the acentric factor and the radius of gyration in the CSP by Mutelet and Rogalski [20]. Nevertheless, despite the meaning of α^{H} and β^{H}, the generalization is not good for associating substances.

In general, none of the equations in Table 4 give good predictions for any particular group of substances (alkanes, benzene derivatives, halogenated alkanes, quantum fluids…), and deviations are high. The three proposed formulas are those in which AAD is less than 15% for most compounds (between 28 and 31 substances), and errors above 100% are less frequent. In the case of Eqs. (44-46), 46 of the 96 compounds have deviations higher than 25%, a good proportion compared with that of Liu et al. (54 of 93) and of Zabaloy et al. (50 of 87). Only for 1,2-dibromotetrafluoroethane the 100% is exceeded, but for this halogenated alkane none of the studied models give reasonable predictions.

Calculated diffusivities of Liu et al. for *n*-triacontane and decamethylcyclopentasiloxane are ten times greater than the real values, such as those obtained for methylcyclohexane with Lee and Thodos. The formula of Zabaloy et al., despite the rejection of experimental points at high densities and low temperatures, has an overall AAD close to that of Ruckenstein and Liu. At low densities (D higher than 10^{-6} m^2s^{-1}) the results of all equations of Table 4 are similar, except for Zhu et al. and for Lee–Thodos: the first one tends to underestimate self-diffusion coefficents while the second one tends to overestimate them considerably.

Figs. 5-7 show the predicted self-diffusivities as a function of the experimental ones of Ruckenstein and Liu, Zhu et al. and Eqs. (44-46). The formula of Ruckenstein and Liu is the best of all those proposed to date, but it tends to underestimate experimental values at high densities. The formula of Zhu and coworkers makes more disperse predictions (in Fig. 6 both underestimations and overestimations can be seen). Only with the mathematical model developed in this work do most of the results fall within ±40% lines.

5. Conclusions

In this paper, self-diffusion coefficients of hard-spheres, Lennard-Jones systems and real fluids have been studied. An empirical interpolation between Chapman-Enskog and the free-volume model of Boned et al. [14] was developed, which is capable to correlate an extensive database in the full-density range.

Concerning real substances, this interpolation can be applied to non-polar, polar, quantic and hydrogen-bonding, with the exception of helium 3, water and hydrogen fluoride. As the model of Boned et al. requires input data measured in relatively wide ranges of temperature and pressure, one of the fitting parameters was generalized (in terms of molar mass, acentric factor, critical temperature and critical volume), making it applicable to data available at few experimental conditions. Nevertheless, this generalization is not valid for hydrogen-bonding molecules.

Finally, all the parameters are expressed as functions of known properties, and the predictive ability of the proposed equation is compared with that of other existing models, obtaining best results with our formulas.

List of symbols

A_D	coupling parameter for diffusion
AAD	average absolute deviation
b_{ji}	empirical coefficient of the equation of Zabaloy et al.
C_1	proportionaly constant in the energy (J m^3 molecule^{-2})
CSP	Corresponding States Principle
D	diffusion (m^2 s^{-1})
f^{corr}	correction function
$g(\sigma)$	radial distribution function
k	Boltzmann constant= 1.380658×10^{-23} J K^{-1}molecule^{-1}
HS	Hard-Sphere
l	length (m)
LJ	Lennard-Jones
LSER	Linear Solvation Energy Relationship
L^{16}	hexadecane-air partition coefficient
M	molar mass (kg mol^{-1})
m	molecular mass (kg molecule^{-1})
N_{atom}	number of atoms in the molecule
NDP	number of data points

OF	objective function
P	pressure (Pa)
R	molecular distance (m)
r_g	radius of gyration (Å)
T	absolute temperature (K)
U	interaction potential energy (J molecule^{-1}), enskog
V	molar volume (m^3 mol^{-1})
V^{free}	free volume (m^3 mol^{-1})
V^{min}	molecular volume (m^3 molecule^{-1})
Z	compressibility factor

Greek letters

α^H	hydrogen-bond acidity
β^H	hydrogen-bond basicity
γ	factor that captures the overlapping of free volumes between molecules
ΔR	excess index of refraction
ε	molecular energy (J molecule^{-1})
η	viscosity (kg m^{-1} s^{-1})
μ_p	dipolar moment (Debye)
ξ	friction coefficient (kg s^{-1})
π'	dipolarity/polarizability of the molecule

ρ	number density, molecules (m^{-3})
σ	molecular diameter (m)
Ω_D	collision integral for diffusion
ω	acentric factor

Superscript

*	molecular reduced parameter
0	low density
calc	calculated
HS	hard-sphere
E	Enskog
eff	effective
exp	experimental
LJ	Lennard-Jones

Subscript

c	critical conditions
f	friction, high-density
r	reduced with respect to the critical point
t	triple point

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Appendix A. Supplementary data

Supplementary Table A1 shows the literature data employed in the present work.

Supplementary Table A2 shows the properties of the substances studied

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FIGURES

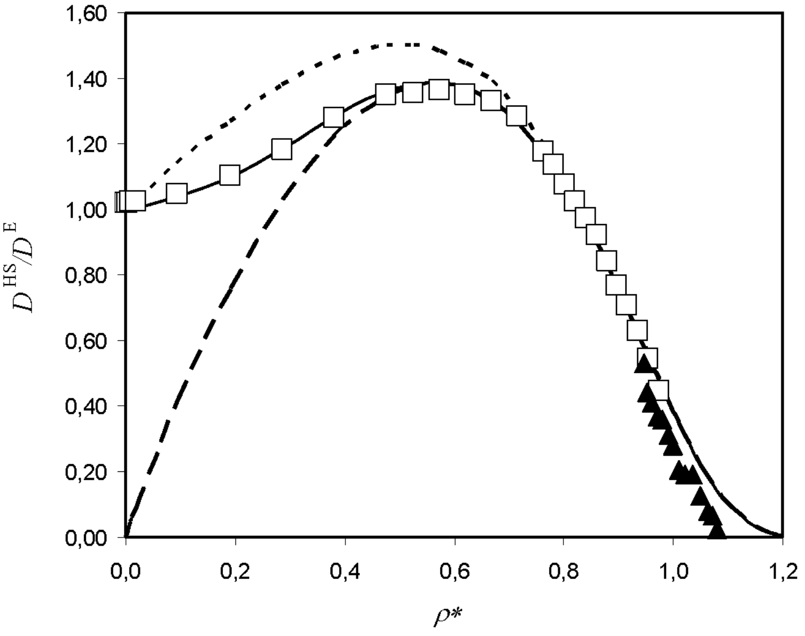

Fig.1. Comparison of Eq. (9) with molecular simulations of hard spheres: (— — — —) original model of Boned et al., (- - - - - - - - - -) with f^{corr} =1.0, (————) with f^{corr} defined by Eq. (10), (□) data of Heyes, (▲) data of Woodcock and Angell.

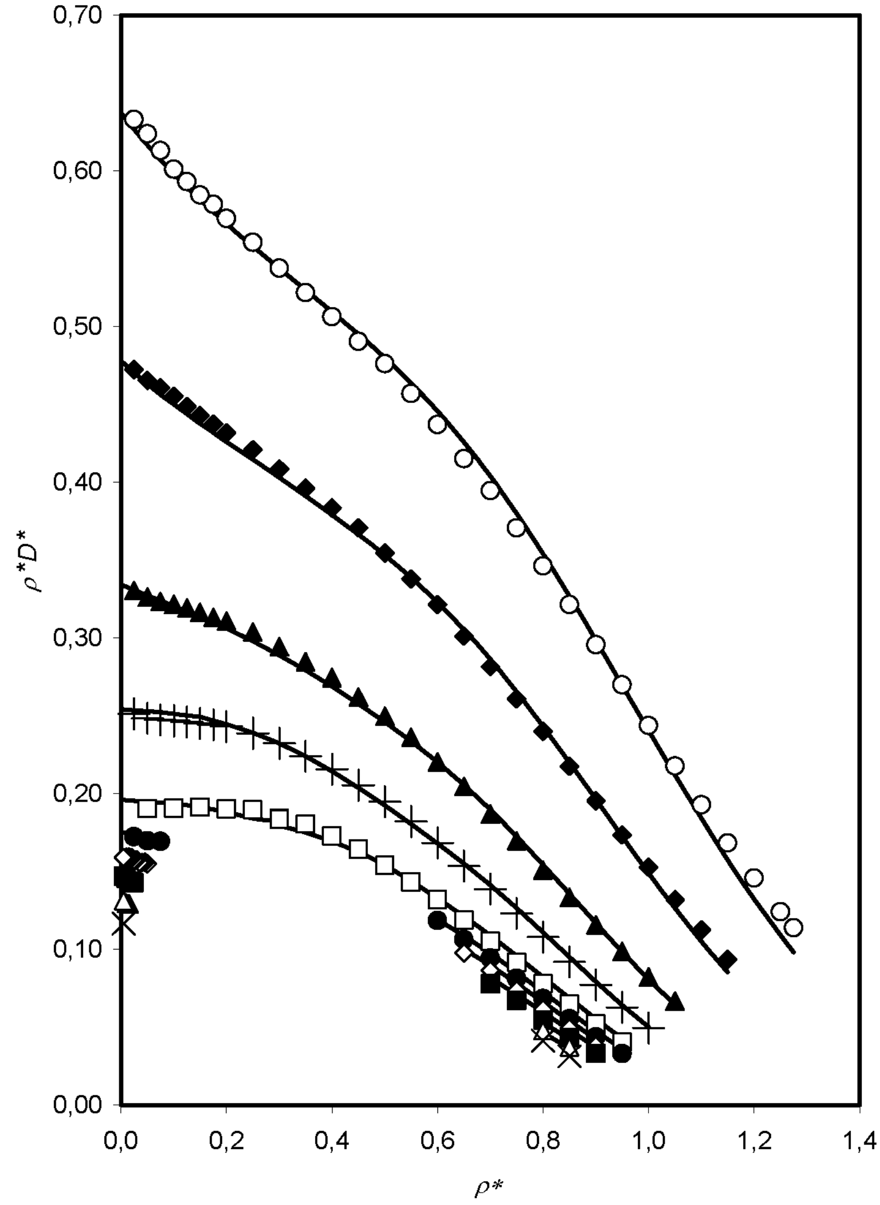

Fig. 2. Density dependence of the group ρ^*D^* according to the molecular simulation of Meier et al. at (×) T^*=0.8, (△) T^*=0.9, (■) T^*=1.0, (◇) T^*=1.1, (●) T^*=1.2, (□) T^*=1.35, (+) T^*=1.8, (▲) T^*=2.5, (◆) T^*=4.0, (○) T^*=6.0. The lines are the results of the correlation with parameters of Table 2.

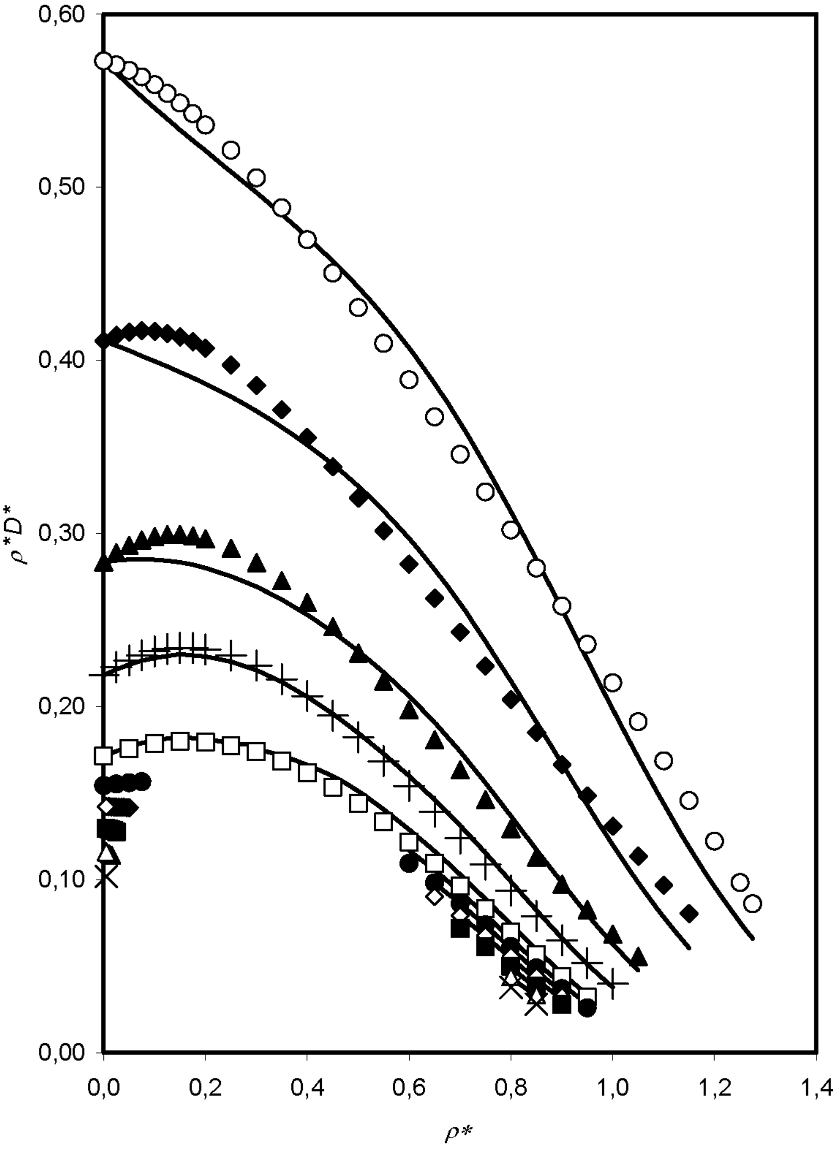

Fig. 3. Density dependence of the group ρ^*D^* according to the molecular simulation of Kataoka and Fujita. Symbols are the same that those of Fig.2. The lines are the results of the correlation with parameters of Table 2.

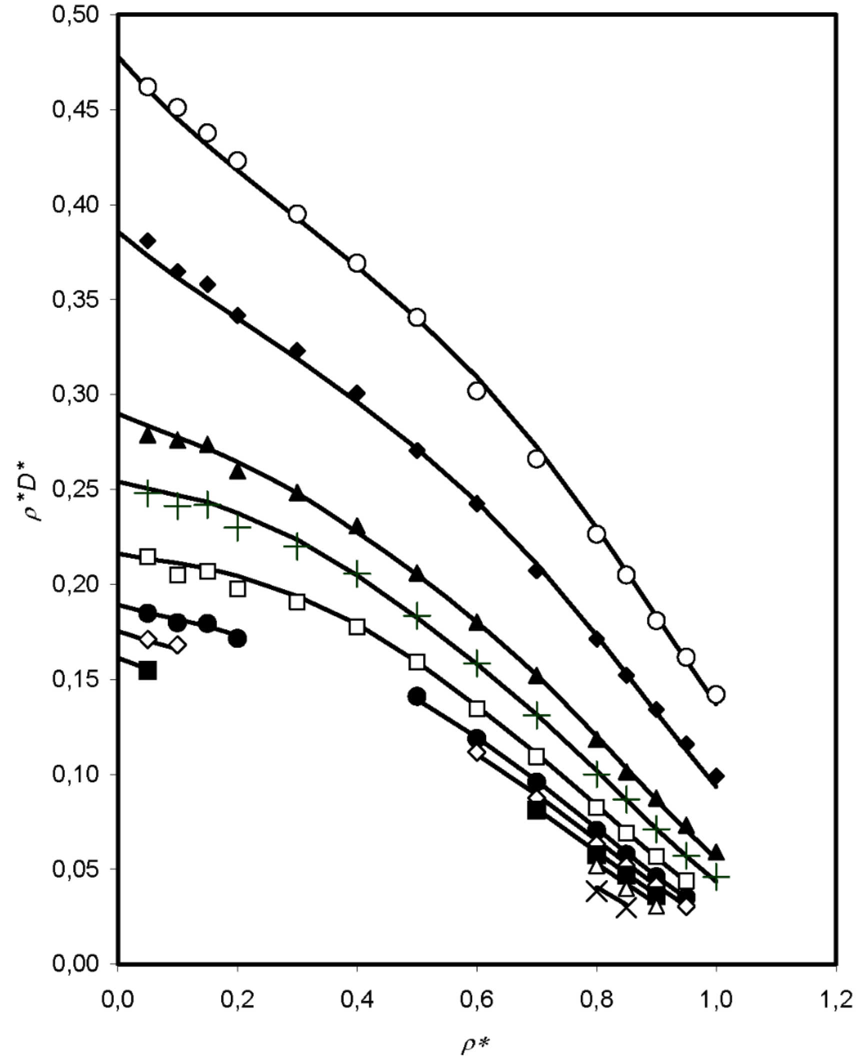

Fig. 4. Density dependence of the group ρ^*D^* according to the molecular simulation of Rowley and Painter at (×) T^*=0.8, (△) T^*=1.0, (■) T^*=1.1, (◇) T^*=1.2, (●) T^*=1.3, (☐) T^*=1.5, (+) T^*=1.8, (▲) T^*=2.1, (◆) T^*=3.0, (○) T^*=4.0. The lines are the results of the correlation with parameters of Table 2.

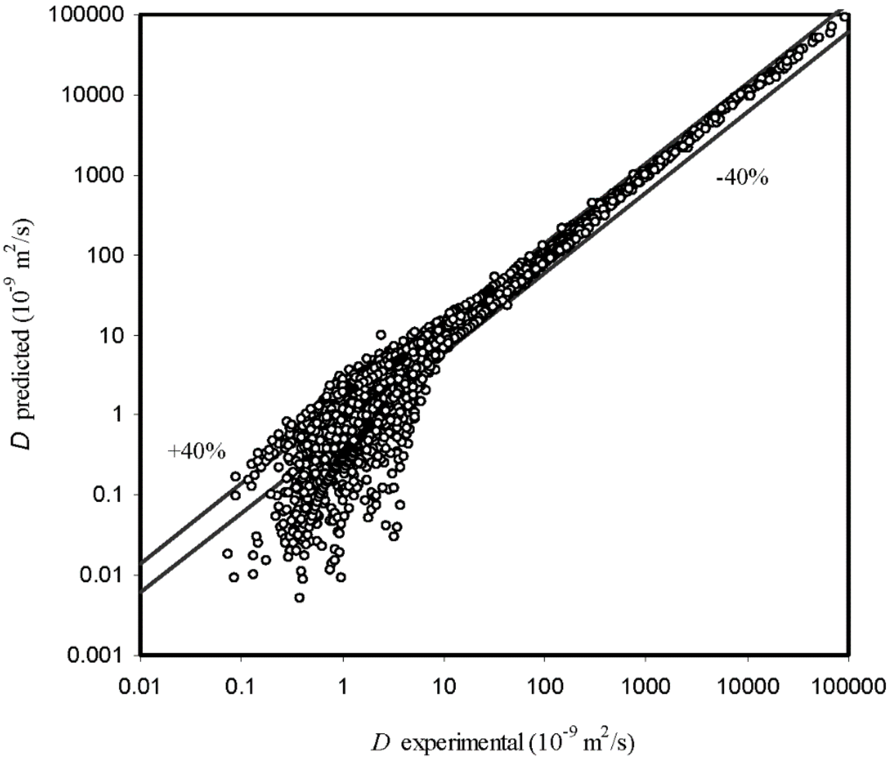

Fig.5. Comparison of experimental self-diffusion coefficients with those predicted by the equation of Ruckenstein and Liu.

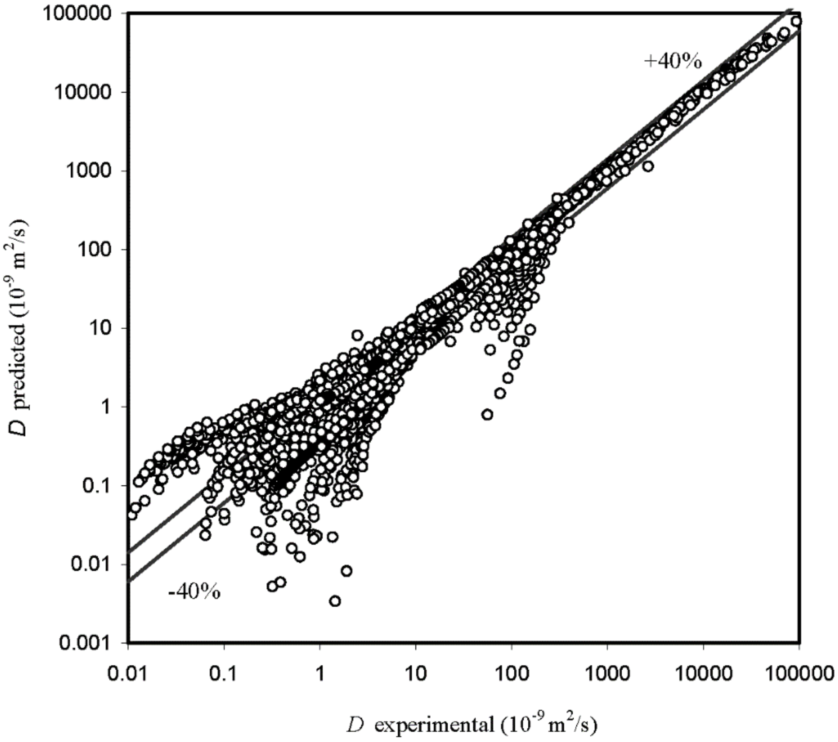

Fig. 6. Comparison of experimental self-diffusion coefficients with those predicted by the equation of Zhu et al.

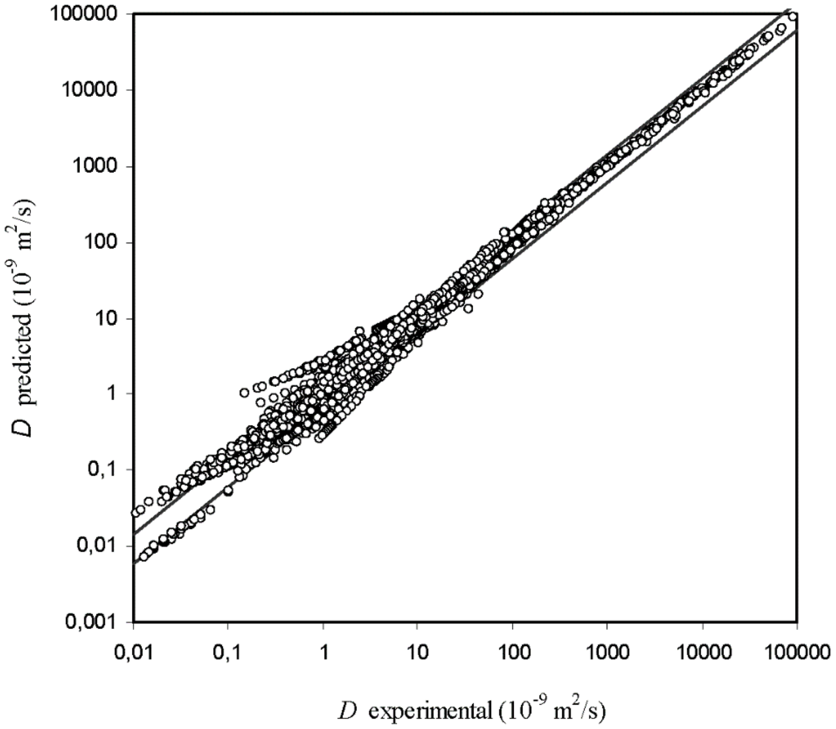

Fig.7. Comparison of experimental self-diffusion coefficients with those predicted by Eqs. (44-46).

TABLES

Table 1

Results of applying Eqs. (9) and (10) to correlate several molecular simulations of hard-spheres

Author	ρ^*	NDP	$ln(l_f^*)$	γ^*	AAD (%)
Heyes et al. [31]	0.0002 – 0.9741	26	-0.51565	0.029288	1.39
Sigurgeirsson and Heyes [32]	0.3820 – 0.9511	13	-0.57376	0.027762	1.24
Erpenbeck and Wood [34]	0.0566 – 0.8839	10	-0.54924	0.027167	0.67
Easteal et al. [35, 36]	0.3535 – 0.9428	19	-0.63657	0.028073	1.03
Alder et al. [37]	0.0141 – 0.9428	8	-0.51905	0.029024	1.93

Table 2

Fitting parameters of Eqs. (8) and (11)

Author	T^*	ρ^*	NDP	$Ln(l_f^*)$	γ^*	C_1^*	AAD (%)
Kataoka and Fujita [38]	0.7 – 6.0	0.000 – 1.275	298	-0.52707	0.023491	8.9557	4.61
Rowley and Painter [39]	0.8 – 4.0	0.050 – 1.000	134	-0.45346	0.018871	10.3433	1.50
Meier et al. [40]	0.7 – 6.0	0.025 – 1.275	282	-0.43801	0.016898	10.0395	2.43

Table 3

Fitting parameters and AAD (%) for self-diffusivities of the compiled substances

SUBSTANCE	NDP	Free fitting of the three parameters				Fitting with C_1* from Eq (44)		
		$ln(l_f*)$	$\gamma*$	C_1*	AAD (%)	$ln(l_f*)$	$\gamma*$	AAD (%)
Methane	403	-0.35934	0.016919	9.5724	5.49	-0.30582	0.016632	5.29
Ethane	83	-0.21994	0.009600	12.6201	5.65	-0.30523	0.009199	5.64
Propane	103	-0.16304	0.008290	14.9852	5.61	-0.17301	0.008405	5.59
n-Butane	34	-0.28203	0.008937	13.8598	5.99	-0.11603	0.006905	7.09
n-Pentane	68	-0.07321	0.008031	15.4269	5.14	0.15568	0.006285	6.80
n-Hexane	134	0.20832	0.006622	19.7286	3.88	0.30238	0.006241	3.98
n-Heptane	74	0.26850	0.007562	19.3348	2.22	0.44925	0.005786	2.71
n-Octane	81	0.50881	0.005513	25.0335	3.56	0.51073	0.005506	3.56
n-Nonane	50	0.80861	0.006022	26.8090	4.20	0.82275	0.005887	4.20
n-Decane	87	0.77275	0.005476	28.2146	7.03	0.81368	0.005272	7.11
n-Dodecane	11					0.82461	0.003888	0.95
n-Tetradecane	35	0.65319	0.003991	31.9118	6.17	0.83531	0.003389	7.16
n-Hexadecane	100	0.92978	0.002417	45.3458	7.64	0.76760	0.002562	7.97
n-Octadecane	22					1.11885	0.002526	4.91
n-Triacontane	63	0.84737	0.001183	75.0201	7.14	0.56646	0.001252	7.60
n-C_{50}	46	1.36317	0.000572	142.5200	6.14	0.54070	0.000660	8.05
n-C_{78}	35	0.86110	0.000315	188.3690	3.66	0.60905	0.000330	3.88
n-C_{154}	24	0.30189	0.000096	329.7790	3.74	0.80848	0.000085	4.60
Neopentane	43	1.18216	0.012221	27.6600	6.09	0.55898	0.019227	8.23
Isopentane	27	-0.24835	0.008639	15.7758	2.04	-0.02137	0.007568	3.57
2,2-Dimethylbutane	31	0.43053	0.014963	17.7170	1.39	0.57720	0.012468	1.91
2,3-Dimethylbutane	22	0.26254	0.007134	21.2841	1.26	0.23202	0.007430	1.28
2-Methylpentane	27	0.14371	0.006940	19.2438	1.37	0.23617	0.006230	1.47
3-Methylpentane	37	0.34210	0.005972	22.2017	2.59	0.27528	0.006512	2.67
2,2,3-Trimethylbutane	25	-0.32249	0.013591	16.0290	2.52	-0.06976	0.009157	7.98
Ethylene	192	-0.31242	0.016544	9.7587	4.09	-0.15403	0.012138	5.67
cis-2-Butene	36	0.17754	0.005442	19.8236	6.55	0.01049	0.006918	6.33
trans-2-Butene	36	0.02772	0.007165	15.0874	6.81	0.12330	0.006331	6.70
Acetilene	37					0.13981	0.030026	0.22
Cyclopentane	30	0.62816	0.009394	22.9172	4.42	0.23933	0.012624	5.69
Cyclohexane	100	0.42175	0.013450	20.1312	4.05	0.33606	0.014344	3.98
Methylcyclohexane	30	0.60910	0.008624	23.3087	8.82	0.37137	0.009433	9.72
Cycloheptane	7					0.41604	0.012897	0.05
Cyclooctane	7					0.51589	0.011099	0.09

SUBSTANCE	NDP	Free fitting of the three parameters				Fitting with C_1* from Eq (44)		
		$ln(l_f*)$	$\gamma*$	C_1*	AAD (%)	$ln(l_f*)$	$\gamma*$	AAD (%)
Cyclodecane	7					0.52228	0.006062	0.13
cis-Decalin	7					0.24998	0.007428	0.08
trans-Decalin	7					0.45744	0.007413	0.03
Bicyclohexane	7					0.93494	0.006106	0.09
Benzene	167	0.27562	0.011503	17.9185	4.41	0.23696	0.011787	4.46
Toluene	72	0.83120	0.007974	22.4638	4.56	0.67163	0.009378	6.36
1,3,5-Trimethylbenzene	70	0.73764	0.007506	22.0761	4.45	0.89630	0.006945	4.73
1,3,5-Triisopropylbenzene	10					0.83270	0.005546	2.70
Dimethyl ether	40	0.03978	0.009327	14.5438	2.49	0.01892	0.009649	2.52
Diethyl ether	6					0.79601	0.010219	3.89
Tetrahydrofurane	12					-0.07780	0.007964	10.20
1,4-Dioxane	10					0.88746	0.021170	2.55
s-Trioxane	4					0.32561	0.014855	0.05
Acetone	52					0.22652	0.009198	5.46
Cyclohexanone	12					0.85817	0.011367	0.33
Pyridine	76	1.04843	0.007917	24.3506	3.67	0.46477	0.010365	9.28
Acetonitrile	68	0.07100	0.008271	14.0881	1.09	0.17375	0.007529	1.51
Trimethylamine	49	0.01525	0.010564	15.1046	4.20	0.12843	0.009189	4.76
N,N-Dimetilformamide	72	0.39070	0.007205	18.5238	5.48	0.42734	0.006915	5.50
N,N -Dimethylacetamide	49	0.38866	0.008771	17.3231	3.80	0.58308	0.006943	4.74
Tetramethylsilane	49	0.00769	0.009017	19.8174	4.51	0.02890	0.008977	4.53
Octamethylcyclotetrasiloxane	21					1.20629	0.006693	6.55
Decamethylcyclopentasiloxane	7					1.09140	0.005123	0.19
Tetramethyl tin	64	-0.14925	0.004946	19.7493	3.01	-0.01623	0.004497	3.52
Fluoromethane	57	-0.10881	0.010597	12.5465	5.84	-0.14480	0.011397	5.91
Fluoroform	114	0.05159	0.010348	15.8531	5.19	-0.09974	0.013027	5.96
Carbon tetrafluoride	137	-0.22047	0.010638	15.5490	8.66	-0.38579	0.012811	9.00
Chloromethane	50	-0.30302	0.009128	12.8480	3.88	-0.28355	0.008777	3.89
Dichloromethane	79	0.17843	0.010125	15.4320	6.06	0.16729	0.010262	6.05
Chloroform	86	-0.02570	0.008279	15.9116	4.01	0.06865	0.007644	4.21
Carbon tetrachloride	50	0.45173	0.014406	18.1817	3.25	0.45382	0.014374	3.27
Chlorodifluoromethane	58	0.12520	0.008651	17.7691	4.08	-0.07577	0.011309	5.41
Chlorotrifluoromethane	131	-0.26640	0.013177	13.2971	6.30	-0.28310	0.010960	7.72
Trichlorofluoromethane	13	-0.10974	0.013660	15.3259	1.69	0.00754	0.012247	1.74
Bromotrifluoromethane	69	-0.35479	0.009512	15.5117	7.37	-0.37785	0.009795	7.37
Dibromomethane	41					0.26824	0.007563	0.26
Iodomethane	5					0.11927	0.009199	0.72

SUBSTANCE	NDP	Free fitting of the three parameters				Fitting with C_1* from Eq (44)		
		$ln(l_f*)$	$\gamma*$	C_1*	AAD (%)	$ln(l_f*)$	$\gamma*$	AAD (%)
Diiodomethane	41					0.68322	0.008729	0.06
1,2-Dichloroethane	23	-0.21463	0.009253	17.3703	3.16	-0.24013	0.009340	3.17
1,2-Dibromotetrafluoroethane	45	-0.77549	0.022552	14.9830	5.06	-0.73272	0.022694	5.43
tert-Butylchloride	21					0.79991	0.019267	7.23
tert-Butylbromide	8					0.16425	0.011952	0.17
Perfluorocyclobutane	59	0.27425	0.021659	17.0599	4.34	0.45743	0.018589	5.04
Fluorobenzene	18					0.51494	0.011272	0.51
Hexafluorobenzene	47	1.09186	0.011871	23.7292	4.18	0.93345	0.013524	4.90
Chlorobenzene	31					0.72963	0.009215	6.48
Bromobenzene	18					0.59806	0.007517	1.80
Iodobenzene	18					0.63980	0.006444	1.09
Trimethylchlorosilane	11					0.20595	0.008104	0.47
Argon	66	-0.57204	0.025642	8.9206	7.09	-0.42887	0.021872	7.32
Krypton	157	-0.02201	0.017769	12.0887	7.63	-0.15896	0.019660	7.84
Xenon	99	-0.02912	0.020589	11.9200	3.58	-0.00423	0.022095	3.81
Oxygen	6							
Nitrogen	21					-0.03580	0.030700	2.65
Carbon monoxide	8					-0.86910	0.003300	6.11
Carbon dioxide	248	-0.23214	0.025551	10.0819	5.67	-0.00664	0.026393	5.10
Sulfur hexafluoride	88	0.21440	0.013167	19.7494	11.47	-0.10860	0.015933	13.16
Carbon disulfide	29	-0.08337	0.006800	13.4974	1.08	0.03395	0.006612	1.25
Hydrogen sulfide	8					-0.01858	0.017042	5.36
Hydrogen	108	-0.47350	0.031134	5.5756	7.03	-0.70690	0.029700	9.59
Deuterium	56	-0.22320	0.055670	6.0695	3.58	-0.22868	0.042650	3.44
Neon	45	-0.35142	0.021219	11.2140	2.64	-0.41884	0.023233	2.58
Helium 3	171							
Water	201							
Heavy water	84							
Ammonia	99	0.29438	0.015324	12.8281	3.27			
Hydrogen fluoride	70							
Methanol	121	2.09109	0.001190	98.2125	5.96			
Ethanol	166	1.49969	0.002445	71.3470	8.02			
1-Propanol	118	2.19753	0.002565	85.4870	3.72			
2-Propanol	68	1.39524	0.009517	38.4015	3.74			
Butanol	3							

SUBSTANCE	NDP	Free fitting of the three parameters				Fitting with C_1* from Eq (44)		
		$ln(l_f*)$	$\gamma*$	C_1*	AAD (%)	$ln(l_f*)$	$\gamma*$	AAD (%)
tert-Butanol	11							
1-Pentanol	85	2.89276	0.002616	92.1868	5.88			
2-Pentanol	39	3.48486	0.002384	115.9089	20.90			
3-Pentanol	45	4.58569	0.002850	120.1553	27.50			
Cyclohexanol	12							
2-Fluoromethanol	30	1.74138	0.005476	45.1421	4.11			
2,2-Difluoromethanol	31	2.11039	0.006085	49.4293	8.89			
2,2,2-Trifluoromethanol	43	1.54730	0.007641	42.9862	6.81			
N-Methyl amine	45	0.23656	0.011529	14.0300	5.95			
N-Methyl formamide	72	0.75963	0.005623	23.6535	3.27			
N-methyl acetamide	34	1.01353	0.005963	30.4612	2.52			
Acetic acid	19							
Pyvalic acid	7							
trifluoracetic acid	7							

Table 4

AAD (%) for several predictive equations

SUBSTANCE	NDP (*)	Eq. (12)	Eq. (19)	Eq. (24)	Eq. (29)	Eq. (36)	Eq. (39)	Eqs. (44-46)	Eqs. (47-49)	Eqs. (50-52)
Methane	403 (383)	7.79	8.22	13.32	20.55	9.58	12.11	5.52	6.88	6.94
Ethane	83 (54)	8.87	6.37	14.70	28.01	12.19	9.43	9.59	10.64	14.93
Propane	103 (42)	24.75	11.02	24.68	25.77	12.77	56.66	16.08	9.19	15.24
n-Butane	34 (13)	26.52	15.17	26.72	22.32	17.40	24.28	19.89	11.25	14.77
n-Pentane	68 (24)	33.38	20.67	31.99	34.87	20.15	21.53	33.91	22.53	22.79
n-Hexane	134 (30)	39.34	17.89	37.95	26.60	25.61	27.13	31.04	18.14	17.31
n-Heptane	74 (29)	40.50	17.55	34.36	37.74	46.58	18.35	34.85	21.27	16.11
n-Octane	81 (17)	41.01	20.74	33.98	26.87	64.52	44.41	30.74	18.00	11.77
n-Nonane	50 (11)	46.92	14.13	36.74	29.31	66.06	53.38	28.70	16.76	13.39
n-Decane	87 (18)	49.47	14.44	37.24	23.87	64.02	72.21	28.69	20.69	14.96
n-Dodecane	11 (6)	62.77	5.83	46.62	40.01	95.40	30.68	41.66	28.30	20.73
n-Tetradecane	35 (6)	83.42	22.60	77.62	52.23	117.56	64.98	40.35	26.84	14.68
n-Hexadecane	100 (8)	94.20	29.03	88.70	68.00	138.23	117.11	27.65	20.52	14.39
n-Octadecane	22 (6)	94.92	81.03	88.78	62.94	165.12	22.84	44.23	38.54	29.82
n-Triacontane	63 (1)	100.00	1432.15	73.93	80.11	268.64		31.41	45.51	
n-C_{50}	46 (0)	100.00		172.72	335.70			49.36		
n-C_{78}	35 (0)	100.00		317.54	575.91			38.13		
n-C_{154}	24 (0)	100.00		505.76	881.41			48.49		
Neopentane	43 (43)	75.40	82.74	79.61	31.20	99.47	60.87	19.50	41.33	52.08

SUBSTANCE	NDP (*)	Eq. (12)	Eq. (19)	Eq. (24)	Eq. (29)	Eq. (36)	Eq. (39)	Eqs. (44-46)	Eqs. (47-49)	Eqs. (50-52)
Isopentane	27 (15)	19.17	33.23	19.41	9.16	40.28	66.87	10.94	5.65	8.29
2,2-Dimethylbutane	31 (10)	71.86	113.42	77.67	34.13	73.41	95.33	15.88	51.06	54.96
2,3-Dimethylbutane	22 (3)	5.87	55.12	10.94	9.17	55.11	60.87	14.53	10.26	11.33
2-Methylpentane	27 (2)	32.62	4.06	29.41	32.56	51.81	42.38	31.53	13.93	10.81
3-Methylpentane	37 (6)	32.79	5.80	31.25	34.58	42.99	30.63	32.25	12.87	10.98
2,2,3-Trimethylbutane	25 (9)	136.79	166.17	142.16	90.11	94.52	223.74	31.73	74.53	87.87
Ethylene	192 (175)	12.68	9.06	15.10	21.81	11.79	8.80	9.36	10.64	10.78
cis-2-Butene	36 (13)	38.64	24.56	40.83	39.31	21.51	14.36	28.46	23.77	
trans-2-Butene	36 (17)	50.92	11.78	53.88	52.82	20.35	50.03	37.86	22.69	
Acetilene	37 (37)	16.93	4.51	19.91	13.23	60.99	8.89	56.44	42.55	47.41
Cyclopentane	30 (15)	42.40	60.18	41.91	16.65	62.94	57.48	13.66	36.01	30.49
Cyclohexane	100 (58)	100.76	127.06	103.19	53.59	143.00	80.24	41.11	81.15	79.33
Methylcyclohexane	30 (0)	63.43	247.55	63.67	197.35		1035.81	67.69	166.09	168.24
Cycloheptane	7 (4)	119.55	142.53	131.51	63.82	176.08	133.34	39.99	90.81	82.96
Cyclooctane	7 (2)	100.06	173.13	107.67	61.62	200.76	110.70	26.49	87.00	86.69
Cyclodecane	7 (1)	85.61	328.21	84.12	24.69	337.87		67.12	93.10	
cis-Decalin	7 (0)	81.39	133.70	96.93	55.88			7.66	67.15	73.07
trans-Decalin	7 (0)	67.66	100.00	82.90	28.56			21.51	30.35	28.37
Bicyclohexane	7 (0)	15.91	35.40	4.90	6.36			22.48	13.72	
Benzene	167 (88)	29.64	17.12	31.22	12.11	54.24	37.21	11.04	20.13	29.64
Toluene	72 (6)	39.06	23.48	38.11	22.56	27.14	87.09	21.61	20.01	16.39
1,3,5-Trimethylbenzene	70 (7)	58.84	49.11	54.18	34.08	36.07	52.18	27.70	20.61	14.13

SUBSTANCE	NDP (*)	Eq. (12)	Eq. (19)	Eq. (24)	Eq. (29)	Eq. (36)	Eq. (39)	Eqs. (44-46)	Eqs. (47-49)	Eqs. (50-52)
1,3,5-Triisopropylbenzene	10 (0)	29.13	94.63	82.48	55.43			12.37	47.90	
Dimethyl ether	40 (21)	23.50	33.50	26.27	35.90	24.33	5.25	15.49	16.39	
Diethyl ether	6 (2)	37.46	43.29	32.05	44.83	4.36	30.33	30.59	25.68	20.62
Tetrahydrofurane	12 (5)	11.11	30.53	13.09	22.60	43.84	87.90	11.70	10.85	11.84
1,4-Dioxane	10 (7)	106.26	48.43	129.47	52.21	123.84	158.25	65.94	77.03	108.98
s-Trioxane	4 (4)	22.43	3.21	35.88	3.47	126.65	43.38	42.42	50.49	
Acetone	52 (24)	53.57	89.01	50.58	52.92	28.88	46.61	12.86	15.50	5.96
Cyclohexanone	12 (5)	29.77	63.92	16.23	21.38	94.76	163.58	78.45	79.16	86.11
Pyridine	76 (19)	32.81	31.02	33.89	27.42	15.38	21.74	17.06	16.34	14.83
Acetonitrile	68 (11)	94.99	100.00	95.35	87.29	25.17	73.04	4.26	25.17	27.47
Trimethylamine	49 (21)	41.39	20.16	45.21	34.52	13.02	38.65	13.83	9.72	5.33
N,N-Dimetilformamida	72 (5)	95.67	99.89	95.74	87.45	41.63	87.97	13.14	20.00	9.73
N,N -Dimethylacetamide	49 (9)	91.03	98.01	91.12	82.46	36.63		21.19	18.21	6.71
Tetramethylsilane	49 (16)	61.00	95.33	50.89	55.33	51.34	103.93	13.08	37.38	
Octamethylcyclotetrasiloxane	21 (12)	54.52	521.80	130.51	118.66	412.61	178.09	31.21	109.07	
Decamethylcyclopentasiloxane	7 (3)	67.43	1045.93	198.88	173.09	499.65	267.14	33.83	123.84	
Tetramethyl tin	64 (26)	22.05	15.06	21.90	25.48	54.17		42.58		
Fluoromethane	57 (46)	43.32	71.74	45.52	51.00	9.87	8.73	6.62	9.39	
Fluoroform	114 (65)	28.16	51.77	28.52	32.28	20.06	16.21	17.90	12.23	
Carbon tetrafluoride	137 (118)	29.84	38.01	34.33	12.98	19.85	54.21	13.97	17.97	22.86
Chloromethane	50 (32)	22.09	33.09	25.25	36.54	13.24	17.64	5.26	5.54	8.49
Dichloromethane	79 (48)	43.75	51.77	45.14	47.68	18.56	14.34	16.60	12.70	7.81

SUBSTANCE	NDP (*)	Eq. (12)	Eq. (19)	Eq. (24)	Eq. (29)	Eq. (36)	Eq. (39)	Eqs. (44-46)	Eqs. (47-49)	Eqs. (50-52)
Chloroform	86 (28)	48.97	12.06	51.71	45.09	20.90	49.03	14.59	16.37	4.24
Carbon tetrachloride	50 (25)	64.77	68.40	64.61	29.26	98.98	70.09	33.56	46.18	63.05
Chlorodifluoromethane	58 (25)	21.97	29.16	23.17	24.42	18.82	31.60	19.94	12.03	
Chlorotrifluoromethane	131 (107)	17.82	27.18	22.17	6.99	19.15		15.83	15.01	
Trichlorofluoromethane	13 (13)	26.12	37.66	23.76	3.74	23.52	44.47	10.55	7.51	
Bromotrifluoromethane	69 (33)	49.39	59.99	44.92	24.41	41.57		14.44	42.08	
Dibromomethane	41 (17)	64.41	14.89	65.66	63.92	14.01	73.41	39.61	22.34	22.26
Iodomethane	5 (1)	55.37	43.66	57.43	58.10	18.67	50.53	36.04	18.74	21.55
Diiodomethane	41 (0)	80.51	99.66	82.25	65.55		50.51	42.84	25.70	27.27
1,2-Dichloroethane	23 (2)	43.49	9.95	49.91	28.88	94.30	108.33	54.92	57.74	73.54
1,2-Dibromotetrafluoroethane	45 (40)	106.48	130.28	77.89	91.29	462.27		201.27	329.84	
tert-Butylchloride	21 (17)	85.50	105.35	91.18	43.29	95.34	61.47	32.47	58.96	67.94
tert-Butylbromide	8 (5)	101.08	233.05	115.49	47.90	126.87		22.68	63.74	83.46
Perfluorocyclobutane	59 (57)	31.40	68.23	40.40	22.33	30.21	45.36	28.11	31.50	
Fluorobenzene	18 (9)	8.08	11.18	9.68	22.12	36.72	26.91	16.59	12.81	13.32
Hexafluorobenzene	47 (29)	13.25	10.86	16.74	18.11	67.23	38.59	22.92	20.30	
Chlorobenzene	31 (14)	31.43	29.81	27.82	40.59	13.74	22.36	34.99	30.30	17.88
Bromobenzene	18 (7)	37.24	38.13	34.12	45.58	14.18	13.31	46.69	28.42	20.59
Iodobenzene	18 (6)	48.77	41.13	46.50	52.67	6.74	14.57	57.98	38.34	30.10
Trimethylchlorosilane	11 (6)	7.68	65.40	7.81	15.37	106.57		10.07	26.34	
Argon	66 (61)	17.14	22.45	35.68	9.52	16.14	12.02	7.87	12.86	11.63
Krypton	157 (156)	11.68	15.09	19.56	12.05	8.77	7.92	11.66	8.89	8.50

SUBSTANCE	NDP (*)	Eq. (12)	Eq. (19)	Eq. (24)	Eq. (29)	Eq. (36)	Eq. (39)	Eqs. (44-46)	Eqs. (47-49)	Eqs. (50-52)
Xenon	99 (99)	6.73	8.16	13.48	20.93	10.76	8.13	19.64	6.37	8.80
Oxygen	6 (5)	4.98	6.19	17.73	9.69	13.13	4.54	6.71	6.56	6.60
Nitrogen	21 (21)	9.16	9.58	9.30	12.27	16.54	10.62	5.91	14.52	9.42
Carbon monoxide	8 (7)	8.93	4.43	6.28	24.72	11.57	25.13	13.20	10.60	9.41
Carbon dioxide	248 (247)	11.77	9.98	18.26	13.80	12.36	6.50	10.12	9.44	8.29
Sulfur hexafluoride	88 (88)	28.60	42.01	48.45	18.64	47.01	42.10	16.31	21.75	23.47
Carbon disulfide	29 (5)	59.49	18.08	62.55	61.52	19.69	60.48	34.33	35.93	49.52
Hydrogen sulfide	8 (7)	15.61	13.67	16.79	40.91	5.66	35.72	7.86	9.96	
Hydrogen	108 (51)	18.27	11.27	26.49	52.36	21.54	56.22	23.16	12.00	15.64
Deuterium	56 (11)	26.38	22.64	36.22	53.05	21.90	62.65	18.65		
Neon	45 (41)	45.85	54.33	39.55	8.37	34.21	11.77	56.24	38.51	40.97
OVERALL	5247 (2898)	39.27	56.96	45.26	44.16	37.36	46.49	22.71	24.61	20.74

(*) Between parenthesis are the number of data that are in the applicability range of Eq. (36)

Table A1

Literature data employed in the present work

SUBSTANCE	NDP	FLUID STATES	SOURCES
Methane	403	All fluid states	[1],[2], [3], [4-11][a]
Ethane	83	Saturated and compressed liquid, dense gas and vapour	[4, 7, 9, 12][b]
Propane	103	Saturated and compressed liquid, dense gas	[4][c,d], [13]
n-Butane	34	Compressed liquid	[14]*
n-Pentane	68	Saturated and compressed liquid	[15-18][c, e, f]
n-Hexane	134	Saturated and compressed liquid	[19], [9,16-18, 20][g]
n-Heptane	74	Saturated and compressed liquid	[21], [15, 16, 22][e], [17][f]
n-Octane	81	Saturated and compressed liquid	[23]; [9, 16,17][c, d]
n-Nonane	50	Saturated and compressed liquid	[16, 22] [e], [17][f]
n-Decane	87	Saturated and compressed liquid	[21], [16, 22][e], [9,17,18][f]
n-Dodecane	11	Atmospheric liquid	[22][e]
n-Tetradecane	35	Saturated and compressed liquid	[22][e], [24][d]
n-Hexadecane	100	Saturated and compressed liquid	[25], [26][d], [22][e]
n-Octadecane	22	Atmospheric liquid	[16, 22][e]
n-Triacontane	63	Compressed liquid	[26][d]
n-C$_{50}$	46	Compressed liquid	[26][h]
n-C$_{78}$	35	Compressed liquid	[26][h]
n-C$_{154}$	24	Compressed liquid	[26][h]
Neopentane	43	Saturated and compressed liquid	[27, 28][i]
Isopentane	27	Saturated and compressed liquid	[29], [30][e]
2,2-Dimethylbutane	31	Saturated and compressed liquid	[17][i]
2,3-Dimethylbutane	22	Saturated and compressed liquid	[17][i]

SUBSTANCE	NDP	FLUID STATES	SOURCES
2-Methylpentane	27	Saturated and compressed liquid	[17][d, e]
3-Methylpentane	37	Saturated and compressed liquid	[17][d]
2,2,3-Trimethylbutane	25	Compressed liquid	[24]*
Ethylene	192	Compressed liquid, dense gas and vapour	[31, 32], [7, 33, 34][j]
cis-2-Butene	36	Compressed liquid	[18][d]
trans-2-Butene	36	Compressed liquid	[18][d]
Acetilene	37	Saturated liquid	[35][e]
Cyclopentane	30	Compressed and atmospheric liquid	[29, 36], [30][e]
Cyclohexane	100	Compressed and saturated liquid	[36-38], [39-43][c]
Methylcyclohexane	30	Compressed liquid	[44]
Cycloheptane	7	Atmospheric liquid	[36]
Cyclooctane	7	Atmospheric liquid	[36]
Cyclodecane	7	Atmospheric liquid	[36]
cis-Decalin	7	Atmospheric liquid	[36]
trans-Decalin	7	Atmospheric liquid	[36]
Bicyclohexane	7	Atmospheric liquid	[36]
Benzene	167	Compressed and saturated liquid	[15, 36, 45-47], [20, 22, 40,48-50][e], [42][l]
Toluene	72	Compressed and saturated liquid	[23], [51, 52][e]
1,3,5-Trimethylbenzene	70	Compressed and saturated liquid	[36, 42, 53]
1,3,5-Triisopropylbenzene	10	Atmospheric liquid	[36]
Dimethyl ether	40	Compressed liquid	[54][m]
Diethyl ether	6	Atmospheric liquid	[51][e]
Tetrahydrofurane	12	Atmospheric liquid	[50, 51][l]
1,4-Dioxane	10	Atmospheric liquid	[15, 55], [50][n]
s-Trioxane	4	Atmospheric liquid	[55]

SUBSTANCE	NDP	FLUID STATES	SOURCES
Acetone	52	Saturated and compressed liquid	[22, 43, 50, 51, 56][o]
Cyclohexanone	12	Saturated liquid	[39][e]
Pyridine	76	Saturated and compressed liquid	[57], [50, 58][e]
Acetonitrile	68	Atmospheric and compressed liquid	[50, 59][p]
Trimethylamine	49	Compressed liquid	[60][e, d]
N,*N*-Dimethylformamide	72	Atmospheric and compressed liquid	[50][e], [61, 62][q]
N,*N* -Dimethylacetamide	49	Compressed liquid	[62][r]
Tetramethylsilane	49	Compressed liquid	[47], [27][p]
Octamethylcyclotetrasiloxane	21	Atmospheric and compressed liquid	[36, 55, 63]
Decamethylcyclopentasiloxane	7	Atmospheric liquid	[36]
Tetramethyl tin	64	Saturated and compressed liquid	[42, 55], [28][n]
Fluoromethane	57	Compressed liquid	[64]
Fluoroform	114	Compressed liquid	[65], [66][n]
Carbon tetrafluoride	137	Saturated and compressed liquid, dense gas	[11][e], [67], [68][s]
Chloromethane	50	Saturated and compressed liquid, dense gas	[69]*
Dichloromethane	79	Saturated and compressed liquid, dense gas	[58, 69, 70][t]
Chloroform	86	Saturated and compressed liquid, dense gas	[71], [69, 72] [t]
Carbon tetrachloride	50	Compressed and saturated liquid	[36, 45, 73], [48][e], [74][n]
Chlorodifluoromethane	58	Compressed liquid, dense gas	[75]*
Chlorotrifluoromethane	131	Saturated and compressed liquid, dense gas	[76], [77][d, u]
Trichlorofluoromethane	13	Compressed liquid	[78]
Bromotrifluoromethane	69	Saturated and compressed liquid, dense gas	[77]*
Dibromomethane	41	Saturated liquid	[70][t]
Iodomethane	5	Saturated liquid	[51][t, v]

SUBSTANCE	NDP	FLUID STATES	SOURCES
Diiodomethane	41	Saturated liquid	[70][w]
1,2-Dichloroethane	23	Compressed liquid	[79]
1,2-Dibromotetrafluoroethane	45	Saturated and compressed liquid	[42]
tert-Butylchloride	21	Saturated liquid	[28, 80][d]
tert-Butylbromide	8	Saturated liquid	[28][w]
Perfluorocyclobutane	59	Dense gas	[81]
Fluorobenzene	18	Atmospheric liquid	[22][e]
Hexafluorobenzene	47	Atmospheric and compressed liquid	[36, 82], [41][n]
Chlorobenzene	31	Saturated liquid	[22, 56][e]
Bromobenzene	18	Atmospheric liquid	[22, 83][e]
Iodobenzene	18	Atmospheric liquid	[22][t, v]
Trimethylchlorosilane	11	Saturated liquid	[28][d]
Argon	66	Compressed and saturated liquid, dense gas and vapour	[84, 85], [5,6, 86-88][c]
Krypton	157	Compressed liquid, dense gas and vapour	[89-92], [6, 93-95][x]
Xenon	99	Compressed and saturated liquid, dense gas and vapour	[6, 96-98][x]
Oxygen	6	Vapour	[5][y]
Nitrogen	21	Saturated liquid, dense gas and vapour	[5, 99, 100][c]
Carbon monoxide	8	Saturated liquid and vapour	[101][e], [102][y]
Carbon dioxide	248	Compressed liquid, dense gas and vapour	[13, 103], [99, 104-106][z]
Sulfur hexafluoride	88	Saturated liquid and vapour, dense gas	[107], [108, 109][e], [110][aa]
Carbon disulfide	29	Compressed liquid	[111]
Hydrogen sulfide	8	Saturated liquid	[112][e]
Hydrogen	108	Saturated and compressed liquid, dense gas and vapour	[113], [114, 115][e], [116, 117][y], [118][bb]
Deuterium	56	Saturated and compressed liquid, dense gas	[115][cc], [118][bb]
Neon	45	Saturated and compressed liquid, vapour	[119][e], [120][e, d, u], [5][y]

SUBSTANCE	NDP	FLUID STATES	SOURCES
Helium 3	171	Saturated and compressed liquid, dense gas and vapour	[121], [122-126][dd]
Water	201	Saturated and compressed liquid, dense gas	[15, 127-130], [42, 131-133][ee]
Heavy water	84	Atmospheric and compressed liquid	[134, 135], [132][n]
Ammonia	99	Saturated and compressed liquid, dense gas and vapour	[136-140][ff]
Hydrogen fluoride	70	Compressed and saturated liquid	[72, 141][e], [142][gg]
Methanol	121	Compressed and saturated liquid	[48, 50, 56, 130, 143][e], [144, 145][hh]
Ethanol	166	Compressed and saturated liquid	[146], [48, 50, 51, 56, 130, 143][e], [144][hh]
1-Propanol	118	Compressed and saturated liquid	[146], [130, 143, 147][e], [148][hh]
2-Propanol	68	Compressed and saturated liquid	[130, 143, 147][e], [148][d]
Butanol	3	Saturated liquid	[143][e]
tert-Butanol	11	Saturated liquid	[28, 143, 147][e]
1-Pentanol	85	Compressed liquid	[149][d, hh]
2-Pentanol	39	Compressed liquid	[149][d, ii]
3-Pentanol	45	Compressed liquid	[149][d, ii]
Cyclohexanol	12	Saturated liquid	[39][e]
2-Fluoromethanol	30	Compressed liquid	[150][d, p]
2,2-Difluoromethanol	31	Compressed liquid	[150][d, p]
2,2,2-Trifluoromethanol	43	Compressed liquid	[150][d, p]
N-Methyl amine	45	Compressed liquid	[60][d, e]
N-Methyl formamide	72	Atmospheric and compressed liquid	[61, 62][d, e]
N-Methyl acetamida	34	Atmospheric and compressed liquid	[62][e, u, w], [151][e]
Acetic acid	19	Atmospheric liquid	[36], [22, 51][e]
Pyvalic acid	7	Atmospheric liquid	[36]
Trifluoracetic acid	7	Atmospheric liquid	[36]

[a] Density or pressure of methane calculated with the equation of state of Setzmann and Wagner [152]

[b] Density or pressure of ethane calculated with the equation of state of Bücker and Wagner [153]

[c] Density or pressure calculated with the equations of state of Span and Wagner [154]

[d] Densities calculated by Hakinson-Brobst-Thomson method [155]

[e] Densities or pressures obtained from Perry and Green [156]

[f] Densities from Cibulka and Hnedkovsky [157]

[g] Density of n-hexane with the equation of state of Harris [19]

[h] Densities of long-chain alkanes from Doolittle and Doolittle [158]

[i] Densities from Cibulka and Takagi [159]

[j] Density or pressure of ethylene calculated with the equation of state of Smukala et al. [160]

[k] Density or pressure of butenes calculated with the equations of state of Lemmon and Ihmels [161]

[l] Densities from Cibulka and Takagi [162]

[m] Density of dimethyl ether calculated with the equation of state of Ihmels and Lemmon [163]

[n] Densities interpolated or extrapolated from data of adjacent references

[o] Densities from Cibulka et al. [164]

[p] Density from Cibulka and Takagi [165]

[q] Densities of N,N-dimethylacetamide from Uosaki et al. [166] and extrapolated with the Hakinson-Brobst-Thomson method [155]

[r] Densities of N,N-dimethylformamide from Easteal and Woolf [61] and extrapolated with the Hakinson-Brobst-Thomson method [155]

[s] Density of carbon tetrafluoride interpolated and extrapolated from Perry et al. [167] and Rubio et al. [168]

[t] Densities from Cibulka et al. [169]

[u] Densities calculated with equations of state from the HYSYS software

[v] Available densities extrapolated with the Rackett method [155]

[w] Densities calculated with Costald method (parameters taken from HYSYS)

[x] Densities calculated with the equations of state of Lemmon and Span [170]

[y] Densities of gases at low pressure

[z] Density of carbon dioxide calculated with the equation of state of Pitzer and Schreiber [171]

[aa] Pressures of sulfur hexafluoride from Keratami et al. [172] and Funke et al. [173]

[bb] Densities from Michels et al. [174]

[cc] Density of saturated liquid deuterium from Chouaieb et al. [175]

[dd] Density of Helium 3 from Huang et al. [176]

[ee] Densities of water calculated with the equation of state of Wagner and Pruβ [177]

[ff] Densities of ammonia calculated with the equation of state of Haar and Gallagher [178]

[gg] Densities of hydrogen fluoride from Karger and Lüdemann [179]

[hh] Densities from Cibulka and Zikova [180]

[ii] Densities from Wappmann et al. [181]

* Graphical reading from the self article and interpolation for non available data.

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Table A2

Properties of the substances whose self-diffusivities have been studied in this work

Substance	Formula	T_c (K)	T_t (K)	$10^{-5}P_c$ (Pa)	T_b (K)	10^6V_c (m^3mol^{-1})	10^3M ($kg\ mol^{-1}$)	ω	r_g (Å)	μ_p (Debyes)	ΔR	π^*	α^H	β^H	*log* L^{16}
Methane	CH_4	190.56	90.69	45.99	111.67	98.63	16.0426	0.01142	1.12300	0.00000	0.000	0.00	0.00	0.00	-0.323
Ethane	C_2H_6	305.33	90.35	48.72	184.55	145.56	30.0694	0.09930	1.83100	0.00000	0.000	0.00	0.00	0.00	0.492
Propane	C_3H_8	369.83	85.48	42.48	231.00	200.00	44.0962	0.15240	2.42600	0.08400	0.000	0.00	0.00	0.00	1.050
n-Butane	C_4H_{10}	425.13	134.90	37.96	272.66	254.92	58.1230	0.20100	2.88900	0.05000	0.000	0.00	0.00	0.00	1.615
n-Pentane	C_5H_{12}	469.70	143.47	33.70	310.98	310.98	72.1498	0.25100	3.38500	0.37000	0.000	0.00	0.00	0.00	2.162
n-Hexane	C_6H_{14}	507.82	177.83	30.34	341.86	369.56	86.1766	0.29900	3.81200	0.05000	0.000	0.00	0.00	0.00	2.668
n-Heptane	C_7H_{16}	540.13	182.55	27.36	371.53	431.91	100.2030	0.34900	4.26700	0.00000	0.000	0.00	0.00	0.00	3.173
n-Octane	C_8H_{18}	569.32	216.38	24.97	398.82	486.29	114.2300	0.39300	4.68000	0.07000	0.000	0.00	0.00	0.00	3.677
n-Nonane	C_9H_{20}	594.55	219.70	22.81	423.97	552.49	128.2570	0.44300	4.98500	0.07000	0.000	0.00	0.00	0.00	4.182
n-Decane	$C_{10}H_{22}$	617.70	243.50	21.03	447.27	609.76	142.2840	0.48800	5.53900	0.07000	0.000	0.00	0.00	0.00	4.686
n-Dodecane	$C_{12}H_{26}$	658.10	263.60	18.17	489.30	751.88	170.3370	0.57400	5.91400	0.00000	0.000	0.00	0.00	0.00	5.696
n-Tetradecane	$C_{14}H_{30}$	693.00	279.01	15.70	526.73	894.00	198.3910	0.58100	6.62100	0.00000	0.000	0.00	0.00	0.00	6.705
n-Hexadecane	$C_{16}H_{34}$	723.00	291.00	14.00	560.01	1034.00	226.4450	0.74200	7.06300	0.00000	0.000	0.00	0.00	0.00	7.714
n-Octadecane	$C_{18}H_{38}$	747.00	301.30	12.90	589.50	1189.00	254.4980	0.79000	7.65500	0.00000	0.000	0.00	0.00	0.00	8.722
n-Triacontane	$C_{30}H_{62}$	863.01		8.68	722.80	1723.53	422.8000	1.30718	8.88500	0.00000					
n-C_{50}	$C_{50}H_{102}$	937.12				2827.70	703.3660	1.90142							
n-C_{78}	$C_{78}H_{158}$	1021.56				4391.99	1096.1220	2.62338							
n-C_{154}	$C_{154}H_{310}$	1149.74				8637.93	2162.1740	4.04011							
Neopentane	C_5H_{12}	433.74	256.60	31.96	282.65	305.81	72.1498	0.16700	3.31800	0.00000	0.000	0.00	0.00	0.00	1.820
Isopentane	C_5H_{12}	460.35	112.65	33.96	300.97	305.72	72.1498	0.22960	3.31300	0.10000	0.000	0.00	0.00	0.00	2.013
2,2-Dimethylbutane	C_6H_{14}	489.00	174.00	31.00	322.88	358.00	86.1766	0.23200	3.47600		0.000	0.00	0.00	0.00	2.352

Substance	Formula	T_c (K)	T_t (K)	$10^{-5}P_c$ (Pa)	T_b (K)	10^6V_c (m^3mol^{-1})	10^3M (kg mol^{-1})	ω	r_g (Å)	μ_p (Debyes)	ΔR	π^*	α^H	β^H	*log* L^{16}
2,3-Dimethylbutane	C_6H_{14}	500.00	145.19	31.50	331.13	361.00	86.1766	0.27400	3.52100		0.000	0.00	0.00	0.00	2.495
2-Methylpentane	C_6H_{14}	497.70	119.55	30.40	333.36	368.32	86.1766	0.28000	3.78400		0.000	0.00	0.00	0.00	2.503
3-Methylpentane	C_6H_{14}	504.60	110.25	31.20	336.42	368.00	86.1766	0.27000	3.69500		0.000	0.00	0.00	0.00	2.581
2,2,3-Trimethylbutane	C_7H_{16}	531.10	160.89	29.50	354.01	398.00	100.2030	0.25000	3.96000	0.00000	0.000	0.00	0.00	0.00	2.918
Ethylene	C_2H_4	282.35	104.00	50.42	169.38	130.94	28.0536	0.08660	1.53800	0.00000	0.107	0.10	0.00	0.07	0.289
cis-2-Butene	C_4H_8	435.75	134.30	42.26	276.87	235.63	56.1072	0.20200	2.83300	0.30000					
trans-2-Butene	C_4H_8	428.61	167.60	42.13	274.03	248.30	56.1072	0.19800	2.80100	0.00000					
Acetilene	C_2H_2	308.30	192.40	61.30	188.43	112.20	26.0378	0.19000	1.09500	0.00000	0.190	0.25	0.21	0.15	0.150
Cyclopentane	C_5H_{10}	511.70	179.28	45.10	322.40	259.00	70.1340	0.19600	3.12000	0.00000	0.263	0.10	0.00	0.00	2.477
Cyclohexane	C_6H_{12}	553.64	279.47	40.75	353.88	308.28	84.1608	0.20926	3.26100	0.30000	0.305	0.10	0.00	0.00	2.964
Methylcyclohexane	C_7H_{14}	572.10	146.58	34.80	374.08	369.00	98.1876	0.23600	3.74700	0.00000	0.244	0.10	0.00	0.00	3.323
Cycloheptane	C_7H_{14}	604.20	265.12	38.20	391.63	353.00	98.1876	0.23700	3.55500		0.350	0.10	0.00	0.00	3.704
Cyclooctane	C_8H_{16}	647.20	287.98	35.60	422.00	410.00	112.2140	0.23600	4.09800		0.413	0.10	0.00	0.00	4.329
Cyclodecane	$C_{10}H_{20}$	667.04		29.65	475.37	569.10	140.2700	0.55826	4.75700						
cis-Decalin	$C_{10}H_{18}$	702.20		32.00	468.60	477.50	138.2500	0.28600	4.50300	0.00000	0.467	0.23	0.00	0.00	4.984
trans-Decalin	$C_{10}H_{18}$	687.00		20.80	460.40	477.50	138.2500	0.27000	4.27300	0.00000	0.544	0.25	0.00	0.00	5.156
Bicyclohexane	$C_{12}H_{22}$	727.00		25.60	512.19	598.00	166.3100	0.42756	4.91700						
Benzene	C_6H_6	562.05	278.69	48.94	353.23	252.77	78.1134	0.20920	3.00400	0.00000	0.610	0.52	0.00	0.14	2.786
Toluene	C_7H_8	591.75	178.18	41.26	383.75	315.56	92.1402	0.26600	3.44300	0.36000	0.601	0.52	0.00	0.14	3.325
1,3,5-Trimethylbenzene	C_9H_{12}	637.30	228.42	31.27	437.89	432.88	120.1940	0.39900	4.34100	0.10000	0.649	0.52	0.00	0.19	4.344
1,3,5-Triisopropylbenzene	$C_{15}H_{24}$	692.87		18.37	511.15	749.50	204.3600	0.53140	5.70600						
Dimethyl ether	$(CH_3)_2O$	400.30	131.65	53.41	248.30	166.31	46.0688	0.20000	2.15400	1.30000	0.000	0.27	0.00	0.41	
Diethyl ether	$(C_2H_5)_2O$	466.74	156.85	36.38	307.60	280.00	74.1224	0.28100	3.14000	1.30000	0.041	0.25	0.00	0.45	2.015
Tetrahydrofurane	C_4H_8O	540.10	164.76	51.90	338.00	224.00	72.1066	0.21700	2.60000	1.70000	0.289	0.52	0.00	0.48	2.636

Substance	Formula	T_c (K)	T_t (K)	$10^{-5}P_c$ (Pa)	T_b (K)	10^6V_c (m^3mol^{-1})	10^3M (kg mol^{-1})	ω	r_g (Å)	μ_p (Debyes)	ΔR	π^*	α^H	β^H	$log\ L^{16}$
1,4-Dioxane	$C_4H_8O_2$	587.00	285.00	52.10	374.60	238.00	88.1060	0.28100	3.11000	0.40000	0.329	0.75	0.00	0.64	2.892
s-Trioxane	$C_3H_6O_3$	604.00	334.20	58.20	387.65	224.00	90.0800	0.33372	2.82300	2.08053					
Acetone	C_2H_6O	508.10	178.50	47.00	329.22	212.76	58.0798	0.30710	2.74000	2.90000	0.179	0.70	0.04	0.51	1.696
Cyclohexanone	$C_6H_{10}O$	653.00	424.00	40.00	428.58	333.00	98.1444	0.44200	3.41000	3.10000	0.403	0.86	0.00	0.56	3.792
Pyridine	C_5H_5N	620.00	231.50	56.70	388.38	243.00	79.1012	0.24300	3.05000	2.30000	0.631	0.84	0.00	0.52	3.022
Acetonitrile	C_2H_3N	545.50	229.32	48.50	354.80	173.00	41.0524	0.32700	1.82100	3.50000	0.237	0.90	0.04	0.33	1.739
Trimethylamine	C_3H_9N	432.79	156.08	40.87	276.02	254.00	59.1108	0.20500	2.73600	0.60000	0.140	0.20	0.00	0.67	1.620
N,*N*-Dimethylformamide	C_3H_7NO	647.00	212.72	44.20	426.15	266.99	73.1000	0.37549	3.02700		0.367	1.31	0.00	0.73	3.173
N,*N* –Dimethylacetamide	C_4H_9NO	657.00		40.20	439.25	321.00	87.1200	0.36350	3.32100		0.363	1.33	0.00	0.78	3.717
Tetramethylsilane	$(CH_3)_4Si$	450.41	182.00	28.14	299.81	357.00	88.2200	0.22400	3.60500	0.00000					
Octamethylcyclotetrasiloxane	$C_8H_{24}Si_4O_4$	586.50	290.25	13.32	448.15	970.00	296.6200	0.58900	6.26000	0.65954					
Decamethylcyclopentasiloxane	$C_{10}H_{30}Si_5O_5$	619.15	226.0	11.60	484.10	1216.00	370.7700	0.66580	7.07400	1.35000					
Tetramethyl tin	$(CH_3)_4Sn$	521.80		29.81	351.00	394.60	178.8300	0.28600							
Fluoromethane	CH_3F	317.28	129.82	58.97	195.03	107.53	34.0331	0.20120	1.41000	1.85100					
Fluoroform	CHF_3	299.29	117.97	48.32	191.13	132.98	70.0141	0.26300	2.45400	1.64900					
Carbon tetrafluoride	CF_4	227.60	86.35	37.40	145.13	140.00	88.0046	0.17700	2.66800	0.00000	-0.280	-0.20	0.00	0.00	-0.800
Chloromethane	CH_3Cl	416.25	175.43	66.79	249.06	139.00	50.4877	0.15300	1.45000	1.90000	0.249	0.43	0.00	0.08	1.163
Dichloromethane	CH_2Cl_2	510.00	178.01	61.00	313.00	185.00	84.9328	0.19900	2.34000	1.80000	0.387	0.57	0.10	0.05	2.019
Chloroform	$CHCl_3$	536.40	209.60	54.70	334.32	239.00	119.3780	0.21800	3.17800	1.10000	0.425	0.49	0.15	0.02	2.480
Carbon tetrachloride	CCl_4	556.60	250.00	45.16	349.90	276.00	153.8230	0.19300	3.45800	0.00000	0.458	0.38	0.00	0.00	2.823
Chlorodifluoromethane	$CHClF_2$	369.30	115.73	49.90	232.34	165.06	86.4687	0.22082	2.05800	1.45800					
Chlorotrifluoromethane	$CClF_3$	302.00		38.79	191.67	179.21	104.4590	0.17230	1.77700	0.51000					
Trichlorofluoromethane	CCl_3F	471.11	162.00	44.08	296.86	247.96	137.3680	0.18875	2.92900	0.45000					
Bromotrifluoromethane	CF_3Br	340.20		39.70	215.26	196.00	148.9100	0.17100	2.26000	0.70000					

Substance	Formula	T_c (K)	T_t (K)	$10^{-5}P_c$ (Pa)	T_b (K)	10^6V_c (m^3mol^{-1})	10^3M (kg mol^{-1})	ω	r_g (Å)	μ_p (Debyes)	ΔR	π^*	α^H	β^H	$log\ L^{16}$
Dibromomethane	CH_2Br_2	611.00	220.60	71.70	370.10	223.00	173.8400	0.20945	2.32700	1.43000	0.714	0.67	0.10	0.10	2.886
Iodomethane	CH_3I	525.00	206.70	65.90	315.70	184.24	141.9400	0.14462	2.35600	1.60000	0.676	0.43	0.00	0.13	2.106
Diiodomethane	CH_2I_2	740.90	279.00	54.20	455.20	267.50	267.8360	0.18000	3.09100		1.453	0.69	0.05	0.23	3.857
1,2-Dichloroethane	$C_2H_4Cl_2$	561.00	237.90	54.00	356.60	225.00	98.9596	0.27800	2.85100	1.80000	0.416	0.64	0.10	0.11	2.573
1,2-Dibromotetrafluoroethane	$C_2Br_2F_4$	487.80		33.93	320.50	341.00	259.8240	0.24500	3.49800						
tert-Butylchloride	$(CH_3)_3CCl$	507.00	247.80	39.50	324.00	295.00	92.5681	0.19000	3.15200	2.10000	0.142	0.25	0.00	0.12	2.217
tert-Butylbromide	$(CH_3)_3CBr$	541.10		43.60	346.40	310.50	137.0300	0.24600	3.55610		0.305	0.25	0.00	0.14	2.616
Perfluorocyclobutane	C_4F_8	388.46	231.80	27.84	267.16	324.00	200.0310	0.35600	3.88800						
Fluorobenzene	C_6H_5F	560.09	234.00	45.51	357.88	269.00	96.1039	0.24400	3.34500	1.40000	0.477	0.57	0.00	0.10	2.788
Hexafluorobenzene	C_6F_6	516.73	278.30	32.73	353.41	335.00	186.0560	0.39600	4.70600						
Chlorobenzene	C_6H_5Cl	632.40	227.60	45.20	404.87	308.00	112.5590	0.24900	3.56800	1.60000	0.718	0.65	0.00	0.07	3.657
Bromobenzene	C_6H_5Br	670.09	242.30	45.20	429.21	324.00	157.0100	0.25100	3.61000	1.50000	0.882	0.73	0.00	0.09	4.041
Iodobenzene	C_6H_5I	721.00	241.80	45.20	461.60	351.00	204.0100	0.24900	3.80800	1.40000	1.188	0.82	0.00	0.12	4.502
Trimethylchlorosilane	$(CH_3)_3SiCl$	497.75		32.00	330.75	366.00	108.6400	0.27012	3.43800	2.08053					
Argon	Ar	150.69	83.81	48.63	87.30	74.59	39.9480	-0.00219	1.07600	0.00000	0.000	0.00	0.00	0.00	-0.688
Krypton	Kr	209.48	115.77	55.25	119.73	92.17	83.8000	-0.00090	1.13760	0.00000	0.000	0.00	0.00	0.00	-0.211
Xenon	Xe	289.73	161.40	58.42	165.05	119.05	131.2900	0.00363	1.29560	0.00000	0.000	0.00	0.00	0.00	0.378
Oxygen	O_2	154.58	54.35	50.43	90.19	73.37	31.9988	0.02220	0.60400	0.00000	0.000	0.00	0.00	0.00	-0.723
Nitrogen	N_2	126.19	63.15	33.96	77.36	89.41	28.0134	0.03720	0.54700	0.00000	0.000	0.00	0.00	0.00	-0.978
Carbon monoxide	CO	132.86	68.15	34.94	81.64	92.17	28.0104	0.05000	0.55800	0.10000	0.000	0.00	0.00	0.00	-0.836
Carbon dioxide	CO_2	304.13	216.55	73.77	194.75	94.12	44.0098	0.22394	0.99200	0.00000	0.150	0.42	0.00	0.10	0.057
Sulfur hexafluoride	SF_6	318.73	222.38	37.54	212.85	196.40	146.0540	0.21000	2.47200	0.00000	-0.600	-0.20	0.00	0.00	-0.120
Carbon disulfide	CS_2	552.00	161.30	79.00	319.00	173.00	76.1310	0.10900	1.42400	0.00000	0.877	0.21	0.00	0.07	2.353
Hydrogen sulfide	H_2S	373.10	187.70	90.00	213.60	98.14	34.0758	0.10000	0.60400	0.97000					

Substance	Formula	T_c (K)	T_t (K)	$10^{-5}P_c$ (Pa)	T_b (K)	10^6V_c (m^3mol^{-1})	10^3M (kg mol^{-1})	ω	r_g (Å)	μ_p (Debyes)	ΔR	π^*	α^H	β^H	*log* L^{16}
Hydrogen	H_2	33.19	13.95	13.15	20.39	66.93	2.0158	-0.21400	0.37100	0.00000	0.000	0.00	0.00	0.00	-1.200
Deuterium	D_2	38.34	18.60	16.65	23.60	57.71	4.0320	-0.17500		0.00000					
Helium 3	He	3.31		1.14	3.19	72.90	3.0170	-0.47300		0.00000					
Neon	Ne	44.49	24.54	26.79	27.10	41.87	20.1790	-0.03870	0.86870	0.00000	0.000	0.00	0.00	0.00	-1.575
Water	H_2O	647.10	273.16	220.64	373.12	55.95	18.0152	0.34430	0.61500	1.85500	0.000	0.45	0.82	0.35	0.260
Heavy water	D_2O	643.89		216.71	374.56	55.94	20.0310	0.36400	0.56800	1.90000					
Ammonia	NH_3	405.40	195.41	113.33	239.82	75.69	17.0304	0.25601	0.85300	1.47000	0.139	0.35	0.14	0.62	0.680
Hydrogen fluoride	HF	461.00	189.79	64.80	293.00	69.00	20.0063	0.32900	0.20000	1.90000					
Methanol	CH_3OH	512.60	175.50	81.04	337.63	116.28	32.0420	0.56250	1.53600	1.70000	0.278	0.44	0.43	0.47	0.970
Ethanol	C_2H_5OH	514.00	159.10	61.37	351.44	168.00	46.0688	0.64400	2.25000	1.70000	0.246	0.42	0.37	0.48	1.485
1-Propanol	C_3H_7OH	536.80	146.90	51.69	370.30	218.00	60.0956	0.62300	2.73600	1.70000	0.236	0.42	0.37	0.48	2.031
2-Propanol	C_3H_7OH	508.30	184.70	47.64	355.40	222.00	60.0956	0.66500	2.72600	1.70000	0.212	0.36	0.33	0.56	1.764
Butanol	C_4H_9OH	563.00	183.90	44.14	390.88	274.00	74.1200	0.59300	3.22500	1.80000	0.224	0.42	0.37	0.48	2.601
tert-Butanol	$(CH_3)_3COH$	506.20	298.80	39.70	355.50	275.00	74.1200	0.61200	3.01900	1.70000	0.180	0.30	0.31	0.60	1.963
1-Pentanol	$C_5H_{11}OH$	588.10	195.56	38.97	411.13	326.00	88.1492	0.57900	3.67900	1.70000	0.219	0.42	0.37	0.48	3.106
2-Pentanol	$C_5H_{11}OH$	552.01	200.00	38.19	392.16	326.99	88.1492	0.67460	3.61900		0.195	0.36	0.33	0.56	2.840
3-Pentanol	$C_5H_{11}OH$	547.01	204.00	38.19	388.46	326.99	88.1492	0.67483	3.50300	1.80000	0.218	0.36	0.33	0.56	2.860
Cyclohexanol	$C_6H_{12}O$	625.00	296.60	37.50	434.40	344.00	100.1600	0.52798	3.60100	1.70000	0.460	0.54	0.32	0.57	3.758
2-Fluoromethanol	C_2H_5FO	551.40		58.22	376.66	183.89	64.0600	0.61615							
2,2-Difluoromethanol	$C_2H_4F_2O$	533.96		51.98	368.66	193.25	82.0500	0.62940							
2,2,2-Trifluoromethanol	$C_2H_3F_3O$	499.29		48.70	347.16	206.69	100.0400	0.63662			0.015	0.60	0.57	0.25	1.224
N-Methyl amine	CH_5N	430.70	179.69	76.14	266.83	154.50	31.0572	0.29200	1.72200	1.30000	0.250	0.35	0.16	0.58	1.300
N-Methyl formamide	C_2H_5NO	720.00		56.20	472.66	215.00	59.0700	0.41000	2.42800		0.405	1.30	0.40	0.55	

Substance	Formula	T_c (K)	T_t (K)	$10^{-5}P_c$ (Pa)	T_b (K)	10^6V_c (m^3mol^{-1})	10^3M (kg mol^{-1})	ω	r_g (Å)	μ_p (Debyes)	ΔR	π^*	α^H	β^H	$log\ L^{16}$
N-Methyl acetamide	C_3H_7NO	718.00	301.15	49.80	478.15	267.00	73.0900	0.43511	3.05100	3.71700	0.400	1.30	0.40	0.72	
Acetic acid	$C_2H_4O_2$	592.71	289.80	57.86	391.00	171.00	60.0520	0.44700	2.59500	1.30000	0.265	0.65	0.61	0.45	1.750
Pyvalic acid	$C_5H_{10}O_2$	632.00		38.90	436.95	336.00	102.1300	0.50927	3.34700	1.70000					
Trifluoracetic acid	$C_2HF_3O_2$	491.30		32.60	346.00	203.97	114.0200	0.54000	3.29400	2.30000					

- Most of T_c, P_c, T_b, V_c, M, ω, r_g and μ_p have been taken from the "Korea thermophysical properties Data Bank", KDB (at website http://www.cheric.org/kdb/), from the "National Institute of Standards and Technology", NIST (http://webbook.nist.gov/chemistry/fluid/) or from the data bank of the software HYSYS.
- Gyration radii of noble gases have been taken from Bosse and Reich [1]. They are usually assumed as zero, but not in this work.
- Dipolar moment of SF_6 and all properties of He^3 and D_2 have been taken from Reid et al. [2]
- T_t were obtained from Lee and Thodos [3,4], Perry and Green [5], the NIST or from the KDB.
- Critical properties and acentric factor of $(CH_3)_4Sn$ were calculated using the method of Rummens and Rajan [6]. The normal boiling temperature was taken from the handbook of Lide [7], and the vapour pressure given in this book has been extrapolated when T_c and P_c were known.
- Critical volume, critical temperature and acentric factors of long-chain alkanes were calculated with the method of Constantinou and Gani, cited by Kontogeorgis and Tassios [8]. In a review, these authors report that it is the best way to obtain these parameters. Nevertheless, the value of the critical pressure when the chain length tends to infinite is not clear: it could be zero or 101.325 Pa.

- Critical properties and normal boiling point of 2,2,2-trifluoroethanol are from Sauermann et al. [9] and the acentric factor has been calculated with the vapour pressure given by these authors. Critical properties of the other fluoroethanols were calculated as the arithmetic mean of the values of two methods: Joback (cited by Reid et al. [2]) and Wen-Qiang [10], because the values obtained for 2,2,2-trifluoroethanol are very close to the experimental ones. The acentric factor given by the equation of Lee-Kesler [2] is acceptable too. Boiling points of 2-fluoroethanol and 2,2-difluoroethanol can be found in the handbook of Lide [7].
- LSER parameters are from Abraham [11] and from Abraham et al. [12]

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