Short communication

Revisiting Tracer Liu-Silva-Macedo model for binary diffusion coefficient using the largest database of liquid and supercritical systems

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Abstract

This work compiles the largest database of tracer diffusion coefficients (D_{12}) containing 6180 experimental points from 331 non-polar and weakly polar liquid and supercritical systems. Then, the Tracer Liu−Silva−Macedo (TLSM) model and its 1-parameter correlations ($TLSM_d$ and $TLSM_{en}$) are evaluated using this database, taking into account the importance of phenomenological and reliable equations for D_{12} estimation. The TLSM model achieves good results with absolute average relative deviations (AARD) of 16.84 % while $TLSM_d$ and $TLSM_{en}$ show better performance with AARD of 4.53 % and 4.55 %, respectively. All properties and parameters needed for D_{12} estimation are compiled in Appendix. For comparison, the models of Wilke-Chang and

Reddy-Doraiswamy, and the correlations of Magalhães *et al*. (LJ-1) and Dymond-Hildebrand-Batschinsky (DHB) are also assessed.

Keywords: Tracer diffusion coefficients; Modeling; Prediction; Correlation; Supercritical fluids; Liquids

1. Introduction

Transport properties, such as viscosity and diffusion coefficient, are essential for the design of equipment and processes involving fluid flow and mass transfer phenomena such as extraction, chromatographic separations and multiphasic reactors [1]. This short communication focuses the diffusion coefficient at infinite dilution, D_{12}, also known as tracer diffusion coefficient. This property is also the basis for the accurate estimation of concentration-dependent diffusivities and the calculation of multicomponent systems, where the Maxwell-Stefan approach is a milestone theory in the area [2,3] in combination with mixing rules like the one proposed by Vignes [4].

The experimental measurement of D_{12} is usually challenging and expensive, mainly in comparison with equilibrium data, which determines the current scarcity of accurate diffusion data. The pure estimation of D_{12} by complementary methods like molecular dynamics (MD) simulations [5] is an alternative, though experimental data is always required to establish/refine the intrinsic MD parameters, calibrate intermolecular potentials, and finally validate the obtained values. Hence the importance of semi-empirical and theoretical/phenomenological expressions for the rigorous calculation of diffusion coefficients is of paramount importance. One may cite: the hydrodynamic predicting equations of Wilke-Chang [6], Scheibel [7], Reddy-Doraiswamy [8], Lusis–

Ratcliff [9], Tyn-Calus [10], Hayduk and Minhas [11], and Lai-Tan [12]; the predicting models of Catchpole-King [13], Zhu *et al.* [14] and Vaz *et al.* [15]; the 2-parameter free-volume correlation of Dymond-Hildebrand-Batschinsky (DHB) [1,16,17]; the 1- and 2-parameter correlations of Magalhães *et al.* [18–21]; and the free-volume hybrid models of Liu and coworkers [1,22] (with 0 and 1 parameter), which rely on the Lennard-Jones (LJ) model previously developed for self-diffusion coefficients [1,23,24].

Liu *et al*. [22] published the Tracer Liu−Silva−Macedo (TLSM) predictive model for D_{12}, based on the seminal LJ fluid model, alongside two 1-parameter correlations ($TLSM_d$ and $TLSM_{en}$), evaluated with 1033 data points spanning 77 liquid and supercritical systems. The TLSM predictive model achieved average absolute relative deviation (AARD) of 14.77 % while the 1-parameter correlations, $TLSM_d$ and $TLSM_{en}$, achieved AARD = 6.57 % and 6.50 %, respectively. Later, Magalhães *et al.* [25] revisited the TLSM model and $TLSM_d$ correlation using a larger database composed of 5279 experimental points from 296 binary systems, including liquid and supercritical systems and also compressed gas systems. The global AARD values achieved were 15.71 % and 3.89 % for TLSM and $TLSM_d$, respectively.

This short communication has two main objectives: (i) Update the D_{12} database, since 72 non-polar liquid and supercritical systems (1323 experimental points) have been reported in last years. In the whole, it includes currently 6180 experimental points spanning 331 binary systems, which makes it the largest D_{12} database published so far. (ii) Revisit the TLSM model and the two derived 1-parameter correlations taking into account they are phenomenological and reliable equations for the calculation of tracer diffusion coefficients. The TLSM, $TLSM_d$ and $TLSM_{en}$ global results are reported along

67 with the results for each individual system and the Lennard-Jones diameter (σ_{LJ}) and
68 energy (ε_{LJ}/k_B) for each pure compound (see Appendix).
69

70 2. Models

71 The predictive TLSM model and the two 1-parameter correlations were assessed
72 with the updated database. For comparison, the Wilke-Chang [6] and Reddy-
73 Doraiswamy [8] predictive models and the correlations of Magalhães *et al*. [20] (LJ-1) and
74 Dymond-Hildebrand-Batschinsky [1,16,17] (DHB) were also tested. These models and
75 correlations are briefly presented in the following.
76

77 *Predictive TLSM model*

78 The predictive TLSM model is described by Equation (1):

$$79 \quad D_{12} = \frac{21.16}{\rho_{n,1}\,\sigma_{eff,12}^2}\left(\frac{1000\,R_g T}{M_{12}}\right)^{1/2} \exp\left(-\frac{0.75\,\rho_1^*}{1.2588-\rho_1^*}-\frac{0.27862}{T_{12}^*}\right) \quad (1)$$

80 where subscripts 1 and 2 indicate the solvent and solute, respectively; T is the absolute
81 temperature (K), R_g is the universal gas constant (8.3144 J mol^{-1} K^{-1}), and $\rho_{n,1}$ is the
82 number density of the solvent ($\rho_{n,1} = \rho_1\,N_{av}/M_1$, where ρ_1 is the density (g cm^{-3}), M_1 the
83 molecular mass (g mol^{-1}) and N_{av} the Avogadro number); M_{12}, T_{12}^* and ρ_1^* are the
84 system's reduced molar mass, temperature and number density defined by Equations
85 (2) – (4); and $\sigma_{eff,i}$ is the effective hard sphere diameter calculated by Equation (5).

$$86 \quad M_{12} = 2\frac{M_1 M_2}{M_1+M_2} \quad (2)$$

$$87 \quad T_{12}^* = \frac{T}{(\varepsilon_{LJ,12}/k_B)} \quad (3)$$

$$\rho_1^* = \rho_{n,1}\sigma_{eff,1}^3 \quad (4)$$

$$\sigma_{eff,i} = \sigma_{LJ,i} \times 2^{1/6}\left(1+\sqrt{1.3229\,T_i^*}\right)^{-1/6},\ i = 1, 12 \quad (5)$$

The binary LJ parameters – the diameter ($\sigma_{LJ,12}$) and energy ($\varepsilon_{LJ,12}/k_B$) – are calculated from the single ones by the combining rules:

$$\sigma_{LJ,12} = \frac{\sigma_{LJ,1}+\sigma_{LJ,2}}{2} \quad (6)$$

$$\frac{\varepsilon_{LJ,12}}{k_B} = \frac{\sqrt{\frac{\varepsilon_{LJ,1}}{k_B}\sigma_{LJ,1}^3 \times \frac{\varepsilon_{LJ,2}}{k_B}\sigma_{LJ,2}^3}}{\sigma_{LJ,12}{}^3} \quad (7)$$

where k_B is the Boltzmann constant (1.380649×10^{-23} J·K^{-1}). Finally, whenever the LJ parameters of any compound are unknown, one can estimate them as function of their critical constants (temperature, T_c, pressure, P_c, and molar volume, V_c) by Equations (8) and (9):

$$\frac{\varepsilon_{LJ,i}}{k_B}(K) = 0.774\,T_{c,i}\text{ , where i} = 1,2 \quad (8)$$

$$\sigma_{LJ,i}^3(Å^3) = 0.17791 + 11.779\frac{T_{c,i}}{P_{c,i}} - 0.049029\left(\frac{T_{c,i}}{P_{c,i}}\right)^2,\ \text{for } \frac{T_{c,i}}{P_{c,i}} \le 100 \quad (9.a)$$

$$\sigma_{LJ,i}(Å) = 0.809\,V_{c,i}^{1/3},\ \text{for } \frac{T_{c,i}}{P_{c,i}} > 100 \quad (9.b)$$

TLSM$_d$ and TLSM$_{en}$ correlations containing 1 parameter

The TLSM$_d$ 1-parameter correlation introduces a binary interaction constant $(k_{12,d})$ in the LJ diameter combining rule. Therefore, Equations (6) and (7) are replaced by:

$$\sigma_{LJ,12} = (1-k_{12,d})\frac{\sigma_{LJ,1}+\sigma_{LJ,2}}{2} \quad (10)$$

$$\frac{\varepsilon_{LJ,12}}{k_B} = 8\frac{\sqrt{\frac{\varepsilon_{LJ,1}}{k_B}\sigma_{LJ,1}^3 \times \frac{\varepsilon_{LJ,2}}{k_B}\sigma_{LJ,2}^3}}{(\sigma_{LJ,1}+\sigma_{LJ,2})^3} \quad (11)$$

The TLSM$_{en}$ 1-parameter correlation introduces the binary interaction constant $\left(k_{12,\mathrm{en}}\right)$ in the LJ energy combining rule. Hence Equation (6) remains the same while Equation (7) is replaced by:

$$\frac{\varepsilon_{\mathrm{LJ},12}}{k_{\mathrm{B}}} = \left(1 - k_{12,\mathrm{en}}\right) \frac{\sqrt{\frac{\varepsilon_{\mathrm{LJ},1}}{k_{\mathrm{B}}} \sigma_{\mathrm{LJ},1}^3 \times \frac{\varepsilon_{\mathrm{LJ},2}}{k_{\mathrm{B}}} \sigma_{\mathrm{LJ},2}^3}}{\left(\sigma_{\mathrm{LJ},12}\right)^3} \tag{12}$$

Wilke-Chang model

The Wilke-Chang equation is described as:

$$D_{12} = \frac{7.4 \times 10^{-8} (\phi M_1)^{1/2} T}{\mu_1 \left(V_{\mathrm{bp},2}^{\mathrm{TC}}\right)^{0.6}} \tag{13}$$

where ϕ is the association factor of the solvent (1.0 for non-associating solvents) and $V_{\mathrm{bp},2}^{\mathrm{TC}}$ the solvent molar volume at normal boiling point, which is estimated in this work by the Tyn-Calus relation:

$$V_{\mathrm{bp,i}}^{\mathrm{TC}} = 0.285 \times V_{\mathrm{c,i}}^{1.048} \tag{14}$$

Reddy-Doraiswamy model

The model is mathematically given by:

$$D_{12} = \beta \frac{T\sqrt{M_1}}{\mu_1 \left(V_{\mathrm{bp},1}^{\mathrm{TC}} V_{\mathrm{bp},2}^{\mathrm{TC}}\right)^{1/3}} \tag{15}$$

where β takes the value of 10×10^{-8} if $V_{\mathrm{bp},1}^{\mathrm{TC}}/V_{\mathrm{bp},2}^{\mathrm{TC}} \leq 1.5$ or 8.5×10^{-8} if $V_{\mathrm{bp},1}^{\mathrm{TC}}/V_{\mathrm{bp},2}^{\mathrm{TC}} > 1.5$. Similarly, to the Wilke-Chang equation, the solvent and solute molar volumes at normal boiling point are estimated by the Tyn-Calus relation (Equation 14).

1-parameter correlation of Magalhães et al. (LJ-1)

The LJ-1 correlation of Magalhães *et al.* [20] for D_{12} of real systems is described by the:

$$D_{12} = \frac{k_B T}{8/3\,\rho_{n,1}\sigma_{eff,12}^2(\pi M_{12} k_B T/N_{av})^{1/2}[g(\sigma_{eff,12})/F_{12}+0.4/T_{12}^{*1.5}]} \quad (16)$$

where M_{12} is the reduced molar mass of the system calculated by Equation (2), $g(\sigma_{12,eff})$ is the pair radial distribution function at contact calculated as proposed by Mansoori *et al*. [26], F_{12} is the correction factor of the hard sphere system calculated as proposed by Magalhães *et al.* [20]. As before, $\sigma_{eff,12}$ is the effective hard sphere diameter but it this calculated by the expression of Ben-Amotz and Herschbach (BAH) according to the Boltzmann criterion [1,27,28]. For simplicity these auxiliary equations are omitted, but can be retrieved from reference [20]. Finally, the adjustable parameter is introduced in the LJ diameter combining rule as shown in Equation (10) for the TLSM$_d$ model.

Dymond–Hildebrand–Batschinski (DHB) 2-parameter correlation

The free volume correlation of Dymond–Hildebrand–Batschinski (DHB) is given by:

$$D_{12} = B_{DHB}\sqrt{T}(V_1 - V_D) \quad (17)$$

where V_1 is the solvent molar volume (cm^3mol^{-1}), and V_D (cm^3mol^{-1}) and B_{DHB} ($cm^{-1}mol\,s^{-1}K^{-1/2}$) are adjustable parameters of the model. V_D is the minimum volume required for diffusion and B_{DHB} is a characteristic constant of the solute-solvent pair.

3. Database

Data used in this work was updated and extended from the database initially published by Magalhães *et al.* [25], being composed of 331 binary systems totalling 6180

151 experimental points, correspondig to 958 diffusivities for 141 liquids systems and 5222
152 diffusivities for 190 supercritical systems. Table A1 (Appendix) lists all systems studied,
153 the sources of data, and the ranges of solvent reduce temperature, T_r, pressure, P_r, and
154 density, ρ_r.

155 Whenever not reported by the original articles, the solvent densities and viscosities
156 were taken from the NIST database [29] or calculated by appropriate equations from
157 Yaws [30] and Przezdziecki and Sridhar [10]. For the particular case of supercritical
158 carbon dioxide (SC-CO_2), densities and viscosities were estimated by the correlations of
159 Pitzer and Schreiber [31] and Altunin and Sakhabetdinov [32], respectively.

160

161 ## 4. Results

162 The results obtained by the predictive TLSM model and its 1-parameter
163 correlations are summarized in Table 1 along with the results for the models and
164 correlations adopted for comparison. Model performance was evaluated in terms of the
165 average absolute relative deviation (AARD) and average relative deviation (ARD)
166 defined by:

167 $$\mathrm{AARD}(\%) = \frac{100}{\mathrm{NDP}} \sum_{\mathrm{i}=1}^{\mathrm{NDP}} \left| \frac{D_{12,\mathrm{i}}^{\mathrm{calc}} - D_{12,\mathrm{i}}^{\mathrm{exp}}}{D_{12,\mathrm{i}}^{\mathrm{exp}}} \right| \quad (18)$$

168 $$\mathrm{ARD}(\%) = \frac{100}{\mathrm{NDP}} \sum_{\mathrm{i}=1}^{\mathrm{NDP}} \frac{D_{12,\mathrm{i}}^{\mathrm{calc}} - D_{12,\mathrm{i}}^{\mathrm{exp}}}{D_{12,\mathrm{i}}^{\mathrm{exp}}} \quad (19)$$

169

170 where NDP refers to the number of experimental points, and superscripts “calc” and
171 “exp” stand for calculated and experimental, respectively. The optimization of all
172 parameters in the case of correlations was always accomplished using AARD as

objective function. Properties and information of all pure components that are necessary for the calculations are compiled in Table A2 (Appendix), namely: name, chemical formula, CAS number, molecular weight, critical temperature, critical pressure, critical volume, and Lennard-Jones force constants (diameter and energy). The detailed results obtained for TLSM, TLSM$_d$ and TLSM$_{en}$ models (*i.e.*, AARD, $k_{12,d}$ and $k_{12,en}$ values) for each individual system are presented in Table A3 (Appendix).

Table 1 – AARD (%) values achieved by the tested models for the diffusion coefficient database (supercritical systems, liquid systems and global averages).

	TLSM	TLSM$_d$	TLSM$_{en}$	Wilke-Chang[ǂ]	Reddy-Doraiswamy[ǂ]	LJ-1	DHB[ǂǂ]
No. of parameters	0	1	1	0	0	1	2
Supercritical (NDP=5222)	16.92	4.25	4.29	14.29	74.67	4.39	4.19
Liquid (NDP=958)	16.44	6.08	6.01	22.91	22.07	7.28	4.42
Global (NDP=6180)	16.84	4.53	4.55	15.64	66.43	4.84	4.23

[ǂ] Only 6118 out of the 6180 experimental points of database were used, due to the lack of necessary properties for the calculation.

[ǂǂ] Only 6176 out of the 6180 experimental points of database were used, because 2 systems only contain 2 diffusivities.

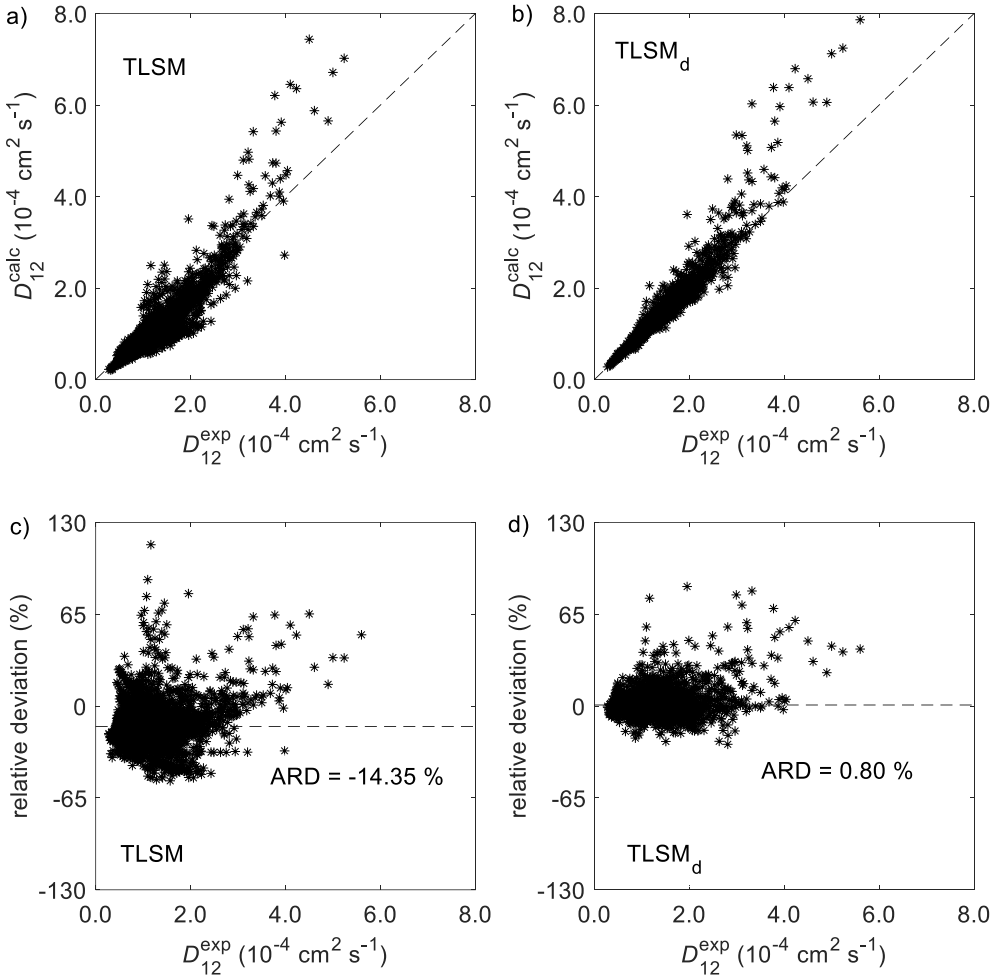
Comparing the AARD results for the predictive TLSM model and its derived 1-parameter correlations, TLSM$_d$ and TLSM$_{en}$, the excellent performance of the latter is

noticeable. To illustrate the improvement achieved by the addition of only one binary interaction parameter, it is shown in Figures 1 and 2 a comparison between TLSM and $TLSM_d$ models for supercritical and liquid systems, respectively, which emphasizes the good and almost unbiased points distribution along ideal expect lines in both cases: D_{12}^{calc} *vs*. D_{12}^{exp} plot, where the expected line is the diagonal, and relative deviation (*i.e.*, non-absolute deviation, *RD*) *versus* D_{12}^{exp} plot, for which the target line is $y = 0$. Similar plots are obtained for $TLSM_{en}$, reason why have been omitted.

In the case of supercritical solvents, when Figures 1a and 1b are compared it is clear that $TLSM_d$ offers a much better distribution of its calculated results along the diagonal, which is coherent with the observed AARD decrease from 16.92 % to 4.25 % (see Table 1). Furthermore, from Figures 1c and 1d it is evident the improvement achieved by $TLSM_d$ in terms of relative deviation taking into account that its average (ARD) jumps from -14.35 % to 0.80 %. Regarding liquid systems, similar conclusions can be drawn based on Figure 2 and Table 1, though the ARD value of TLSM is already very low (-0.27 %) and increases a little in the case of $TLSM_d$ (ARD = -1.58 %). It is worth noting this occurs because the objective function adopted to fit parameter $k_{12,d}$ is AARD instead of ARD. Nonetheless, the gain in terms of AARD is notorious, as it decreases from 16.44 % (TLSM) to 6.08 % ($TLSM_d$).

The results achieved by the predictive models (see Table 1) evidences the poor behavior of the Reddy-Doraiswamy equation with an overall AARD of 66.43 %, in particular for the supercritical fluid systems where AARD = 74.67 %. The well-known Wilke-Chang model shows an overall good performance (AARD = 15.64 %), slightly better than the TLSM model (AARD = 16.84 %). However, when comparing separately

211 the liquid and supercritical systems it can be seen that the D_{12} for liquids seems to be
212 better translated by the TLSM model with an AARD 6.47 % lower than the one achieved
213 by the Wilke-Chang equation. Regarding the supercritical systems the opposite is
214 verified, with the TLSM model exhibiting and AARD value 2.63 % higher than the Wilke-
215 Chang equation. Noteworthy, the AARD results achieved by the TLSM model are more
216 coherent between the supercritical and liquid systems than the Wilke-Chang equation –
217 a difference of only 0.48 % is observed for the former and a difference of 8.63 % is
218 observed for the latter. Regarding the 1-parameter correlations $TLSM_d$ and $TLSM_{en}$, the
219 results achieved for both are similar with global AARD values of 4.53 % and 4.55 %,
220 respectively. These results are very close to those achieved by the DHB equation (AARD
221 = 4.23 %) and the 1-parameter LJ-1 correlation (AARD = 4.84 %) even though the DHB
222 model embodies two adjustable parameters. It should also be noted that, in the case of
223 liquid systems, the DHB correlation shows a better performance than the remaining
224 correlations albeit their overall good performance (AARD < 7.28 %).



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226 Figure 1 – Results achieved by TLSM and TLSM$_d$ models for supercritical systems: (a) calculated *versus*
227 experimental diffusion coefficients (D_{12}^{calc} *vs.* D_{12}^{exp}) of TLSM; (b) D_{12}^{calc} *vs.* D_{12}^{exp} of TLSM$_d$; (c) relative deviation
228 *vs.* D_{12}^{exp} for TLSM; (d) relative deviation *vs.* D_{12}^{exp} for TLSM$_d$. In subplots (c) and (d) the horizontal dashed
229 line (---) represents the average relative deviation (ARD).

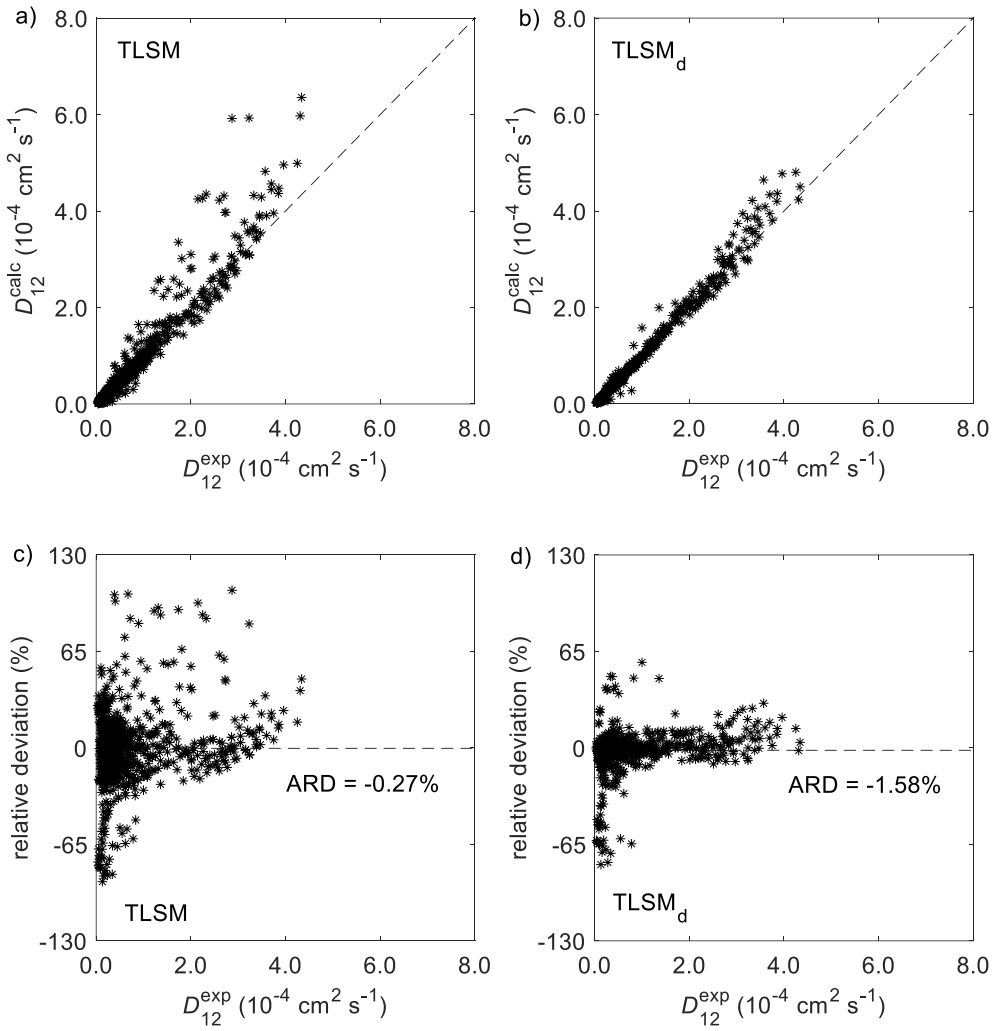

Figure 2 – Results achieved by TLSM and TLSM$_d$ models for liquid systems: (a) calculated *versus* experimental diffusion coefficients (D_{12}^{calc} *vs.* D_{12}^{exp}) of TLSM; (b) D_{12}^{calc} *vs.* D_{12}^{exp} of TLSM$_d$; (c) relative deviation (RD) *vs.* D_{12}^{exp} for TLSM; (d) relative deviation *vs.* D_{12}^{exp} for TLSM$_d$. In subplots (c) and (d) the horizontal dashed line (---) represents the average relative deviation (ARD).

5. Conclusions

In this work it is compiled the largest database of tracer diffusion coefficients, containing 6180 experimental points spanning 331 non-polar liquid and supercritical systems. Additionally, the Tracer Liu-Silva-Macedo (TLSM) model and its 1-parameter

240 correlations ($TLSM_d$ and $TLSM_{en}$) were reassessed using this enlarged database. The
241 predictive TLSM model exhibits good results (global AARD of 16.84 %) being slightly
242 worse than the Wilke-Chang model and significantly better than the Reddy-
243 Doraiswamy model. Nevertheless, the TLSM model is the best option to estimate D_{12} in
244 liquid systems (AARD = 16.44 %) and it is the most trustworthy model for D_{12} prediction,
245 since it exhibits an equivalent performance for both liquid and supercritical fluids (16.44
246 % and 16.92 %). Regarding the $TLSM_d$ and $TLSM_{en}$ 1-parameter correlations, the global
247 AARD values are low (4.53 % and 4.55 %, respectively) and very similar to those
248 achieved by Magalhães *et al*. (LJ-1) (AARD = 4.84 %; 1-parameter) and Dymond-
249 Hildebrand-Batschinsky (DHB) (AARD = 4.23 %; 2-parameters). In Appendix are
250 collected all properties and parameters needed for the calculation of D_{12}.
251

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257

258 **Nomenclature**

ARD	Average relative deviation
AARD	Average absolute relative deviation
B_{DHB}	Characteristic constant of the solute-solvent pair from the DHB correlation
D_{12}	Tracer diffusion coefficient

DHB	Dymond-Hildebrand-Batchinski
F_{12}	Correction factor of the hard sphere system
$g(\sigma_{12,\mathrm{eff}})$	Pair radial distribution function at contact
LJ	Lennard-Jones
LJ-1	D_{12} correlation by Magalhães *et al*. [20]
M_{12}	Reduced molecular weight
M_{i}	Molecular weight of the component i
N_{av}	Avogadro number
NDP	Number of data points
$k_{12,\mathrm{d}}$	Binary interaction constant of the TLSM$_{\mathrm{d}}$ correlation
$k_{12,\mathrm{en}}$	Binary interaction constant of the TLSM$_{\mathrm{en}}$ correlation
k_{B}	Boltzmann constant (1.380649×10^{-23} J·K^{-1})
P_c	Critical pressure
R_{g}	Universal gas constant (8.3144 J mol^{-1} K^{-1})
T	Absolute temperature
T_c	Critical temperature
T_{i}^{*}	Reduced temperature
TLSM	Tracer Liu-Silva-Macedo
TLSM$_{\mathrm{d}}$	Tracer Liu-Silva-Macedo 1-parameter correlation (diameter)
TLSM$_{\mathrm{en}}$	Tracer Liu-Silva-Macedo 1-parameter correlation (energy)
$V_{\mathrm{bp,i}}^{\mathrm{TC}}$	Molar volume at normal boiling temperature estimated by the Tyn-Calus relation
V_{c}	Critical molar volume

V_{D}	Minimum volume required for diffusion from the DHB correlation
V_1	Solvent molar volume

Greek letters

β	Constant from the Reddy-Doraiswamy model
$\varepsilon_{\mathrm{LJ,i}}/k_{\mathrm{B}}$	Lennard Jones energy of the component i
μ_1	Solvent viscosity
ρ_1	Solvent density
$\rho_{\mathrm{n},1}$	Solvent number density
ρ_1^*	Reduced number density of the solvent
$\sigma_{\mathrm{LJ,i}}$	Lennard Jones diameter of component i
$\sigma_{\mathrm{eff,i}}$	Effective hard sphere diameter of component i
ϕ	Association factor

Subscripts

1	Solvent
2	Solute
12	Solute-solvent pair
c	Critical property
r	Reduced property (using critical constants)

Superscripts

calc	Calculated

exp	Experimental
*	Reduced property (using LJ constants)

259

Appendix

Table A1 – Systems studied, reduce temperature, T_r, pressure, P_r, and density, ρ_r, in relation to solvent. Source of the diffusion data.

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
carbon dioxide	acetone	213	0.997-1.096	1.076-5.435	0.772-2.076	[33–37]
	acridine	6	1.013-1.079	2.337-3.734	1.515-1.956	[38]
	adamantanone	8	1.031	1.355-2.033	1.330-1.662	[39]
	allylbenzene	15	1.030-1.096	2.033-4.743	1.295-1.997	[40]
	aluminum acetylacetonate	84	1.013-1.096	1.057-5.420	0.707-2.074	[41]
	aniline	15	1.030-1.096	2.033-4.743	1.296-1.910	[42]
	anisole	15	1.029-1.095	2.033-4.743	1.296-1.997	[43]
	anthracene	22	1.029-1.095	14.499-47.425	0.768-1.995	[44]
	arachidonic acid (AA)	75	1.013-1.128	1.287-4.131	1.188-1.989	[45]
	AA ethyl ester	48	1.013-1.112	1.141-4.058	1.068-1.816	[46]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	behenic acid ethyl ester	17	1.013-1.046	1.310-2.852	1.280-1.814	[47]
	benzene	249	0.997-1.096	1.084-4.743	0.595-1.996	[34,48–55]
	benzoic acid	35	0.964-1.079	0.962-4.065	1.146-1.956	[13,38,56,57]
	benzyl acetate	15	1.030-1.096	2.033-4.743	1.295-1.997	[58]
	benzylacetone	15	1.030-1.096	2.033-4.743	1.295-1.997	[59]
	biphenyl	24	0.964-1.063	0.962-2.317	1.148-1.946	[57]
	2-bromoanisole	15	1.030-1.096	2.033-4.743	1.295-1.997	[40]
	bromobenzene	21	1.029-1.095	2.033-4.743	1.296-1.997	[60,61]
	2-butanone	40	1.013-1.079	1.129-4.679	1.243-2.029	[35,61,62]
	N-(4-methoxybenzylidene)-4-*n*-butylaniline	5	1.031	1.626-2.168	1.527-1.694	[39]
	n-butylbenzene	15	1.029-1.095	2.033-4.743	1.295-1.997	[63]
	sec-butylbenzene	15	1.029-1.095	2.033-4.743	1.295-1.997	[64]
	tert-butylbenzene	15	1.029-1.095	2.033-4.743	1.296-1.997	[65]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	butyric acid ethyl ester	16	1.013-1.046	1.310-2.852	1.280-1.814	[66,67]
	caffeine	25	1.013-1.096	1.088-2.285	0.920-1.723	[68–70]
	capric acid ethyl ester	16	1.013-1.046	1.310-2.852	1.280-1.814	[66,67]
	caprylic acid ethyl ester	16	1.013-1.046	1.310-2.852	1.280-1.814	[66,67]
	β-carotene	90	1.013-1.096	1.236-4.111	1.335-1.987	[71–73]
	L-carvone	27	1.013-1.112	2.033-4.065	1.389-1.984	[74,75]
	chlorobenzene	21	1.029-1.095	2.033-4.743	1.296-1.997	[60,61]
	chromium(III) acetylacetonate	104	1.013-1.128	1.098-5.420	0.859-2.076	[76,77]
	chrysene	4	0.997-1.096	2.168-3.591	1.707-1.878	[34]
	citral	15	1.030-1.096	1.626-2.710	0.953-1.799	[78]
	cobalt(III) acetylacetonate	38	1.030-1.096	1.314-5.420	1.288-2.041	[79]
	copper(II) trifluoroacetylacetonate	12	1.013-1.046	1.466-2.243	1.284-1.759	[80]
	15-crown-5	29	1.013-1.030	1.188-4.070	0.900-1.943	[81]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	dibenzo-24-crown-8	28	1.013-1.030	2.034-4.743	1.666-2.024	[81]
	cycloheptanone	8	1.033-1.033	1.355-2.439	1.297-1.738	[82]
	cyclononanone	8	1.033-1.033	1.355-2.439	1.297-1.738	[82]
	cyclopentanone	8	1.033-1.033	1.355-2.439	1.297-1.738	[82]
	n-decane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	dibenzyl ether	15	1.030-1.096	2.033-4.743	1.295-1.997	[58]
	1,2-dichlorobenzene	15	1.029-1.095	2.033-4.743	1.296-1.997	[65]
	1,3-dichlorobenzene	4	1.030	2.033-3.252	1.667-1.863	[74]
	p-dichlorobenzene	13	0.980-1.046	1.252-2.317	1.148-1.867	[57]
	diethyl ether	17	1.030-1.096	1.084-2.168	0.418-1.704	[61,62,84]
	1,2-diethylbenzene	15	1.030-1.096	2.033-4.743	1.295-1.997	[85]
	1,4-diethylbenzene	15	1.030-1.096	2.033-4.743	1.295-1.997	[85]
	diisopropyl ether	15	1.030-1.096	1.084-2.168	0.418-1.704	[84]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	2,3-dimethylaniline	15	1.029-1.095	2.033-4.743	1.296-1.997	[86]
	2,6-dimethylaniline	15	1.029-1.095	2.033-4.743	1.296-1.997	[86]
	1,1′-dimethylferrocene	68	1.013-1.063	1.114-5.436	0.828-2.077	[87]
	2,3-dimethylnaphthalene	3	1.013-1.013	1.341-2.629	1.513-1.837	[88]
	2,6-dimethylnaphthalene	6	1.013-1.013	1.233-2.642	1.427-1.839	[88,89]
	2,7-dimethylnaphthalene	6	1.013-1.013	1.450-2.710	1.571-1.848	[88,89]
	2,4-dimethylphenol	15	1.029-1.095	2.033-4.743	1.296-1.997	[43]
	diolein	9	1.030	1.355-3.389	1.341-1.878	[90]
	disperse blue 14	47	1.019-1.052	2.710-4.607	1.758-1.980	[91]
	disperse orange 11	65	1.013-1.079	2.710-5.420	1.689-2.041	[91]
	1,3-divinylbenzene	15	1.030-1.096	2.033-4.743	1.295-1.997	[40]
	docosahexaenoic acid (DHA)	63	1.013-1.128	1.256-4.083	1.219-1.985	[92]
	DHA ethyl ester	65	1.013-1.112	1.141-4.058	1.069-1.816	[46,47]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	DHA methyl ester	17	1.013-1.046	1.310-2.852	1.280-1.814	[47]
	n-dodecane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	eicosapentaenoic acid (EPA)	55	1.013-1.128	1.176-4.085	1.157-1.951	[92]
	EPA ethyl ester	48	1.013-1.112	1.141-4.058	1.068-1.816	[46]
	EPA methyl ester	17	1.013-1.046	1.310-2.852	1.280-1.814	[47]
	ethanol	24	1.030	1.287-3.388	1.236-1.878	[56]
	ethyl acetate	16	1.013-1.079	1.024-2.168	0.456-1.723	[62,68]
	ethyl benzoate	15	1.030-1.096	2.033-4.743	1.295-1.997	[59]
	ethylbenzene	15	1.030-1.096	2.033-4.743	1.295-1.997	[50]
	2-ethyltoluene	15	1.029-1.095	2.033-4.743	1.296-1.910	[93]
	3-ethyltoluene	15	1.029-1.095	2.033-4.743	1.296-1.910	[93]
	4-ethyltoluene	15	1.029-1.095	2.033-4.743	1.296-1.910	[93]
	eugenol	15	1.030-1.096	2.033-4.743	1.295-1.997	[59]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	ferrocene	107	1.013-1.096	1.087-5.466	0.600-2.077	[87,94]
	2-fluoroanisole	15	1.030-1.096	2.033-4.743	1.295-1.997	[40]
	fluorobenzene	15	1.029-1.095	2.033-4.743	1.296-1.910	[60]
	3-fluorophenol	4	1.030	2.033-3.252	1.667-1.863	[74]
	geraniol	4	1.030	2.033-3.252	1.667-1.863	[74]
	n-heptane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	2-heptanone	11	1.034-1.034	1.423-2.439	1.364-1.734	[39]
	4-heptanone	9	1.031	1.355-2.168	1.330-1.694	[39]
	hexachlorobenzene	14	1.013-1.079	1.310-3.352	0.870-1.922	[95]
	1-hexadecene	11	1.030-1.227	1.355-4.065	0.913-1.943	[96]
	1,1,1,5,5,5-hexafluoroacetylacetone	15	1.013-1.046	1.411-3.008	1.210-1.870	[80]
	n-hexane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	ibuprofen	99	1.013-1.161	1.152-5.420	0.927-2.074	[97]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	iodobenzene	20	1.029-1.095	2.033-4.743	1.296-1.997	[60,61]
	isobutylbenzene	15	1.029-1.095	2.033-4.743	1.295-1.997	[64]
	D-limonene	15	1.030-1.096	1.626-2.710	0.953-1.799	[78]
	linalool	15	1.030-1.096	1.626-2.710	0.953-1.799	[48]
	linoleic acid	71	1.013-1.128	1.152-4.106	1.188-1.987	[45]
	linoleic acid methyl ester	20	1.013-1.079	1.897-4.553	1.577-1.982	[98,99]
	α-linolenic acid	56	1.013-1.128	1.152-4.084	1.163-1.984	[92]
	γ-linolenic acid	142	1.013-1.128	1.176-4.133	0.976-1.948	[100]
	γ-linolenic acid ethyl ester	41	1.030-1.128	1.138-2.169	0.716-1.697	[100]
	γ-linolenic acid methyl ester	52	1.030-1.128	1.099-4.553	0.622-1.982	[98,100]
	L-menthone	23	1.013-1.112	2.033-4.065	1.389-1.984	[75]
	methanol	10	1.030	1.287-2.846	1.236-1.812	[56]
	2-methylanisole	15	1.029-1.095	2.033-4.743	1.296-1.997	[86]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	4-methylanisole	15	1.029-1.095	2.033-4.743	1.296-1.997	[86]
	3-methylbutylbenzene	15	1.029-1.095	2.033-4.743	1.295-1.997	[64]
	1-methylnaphthalene	11	1.030-1.227	1.355-4.065	0.913-1.943	[96]
	monoolein	11	1.030	1.356-3.388	1.343-1.878	[90]
	myristic acid ethyl ester	16	1.013-1.046	1.310-2.852	1.280-1.814	[66,67]
	myristoleic acid	42	1.030-1.128	1.247-4.065	0.977-1.878	[101]
	myristoleic acid methyl ester	81	1.030-1.128	1.084-3.388	0.481-1.878	[101,102]
	naphthalene	114	0.948-1.096	0.911-13.550	0.470-2.374	[34,70,88,94,103]
	1-naphthol	11	1.013-1.046	1.436-2.195	1.131-1.745	[44]
	2-naphthol	16	1.013-1.079	1.341-2.060	0.702-1.718	[44]
	2-nitroanisole	15	1.029-1.095	2.033-4.743	1.296-1.997	[65]
	nitrobenzene	23	1.029-1.095	2.033-4.743	1.296-1.997	[43,61]
	3-nitrotoluene	15	1.029-1.095	2.033-4.743	1.296-1.997	[86]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	n-nonane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	2-nonanone	10	1.034-1.034	1.355-2.033	1.282-1.646	[39]
	5-nonanone	12	1.034-1.034	1.355-2.439	1.282-1.734	[39]
	n-octane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	oleic acid	19	1.030	1.282-4.079	1.225-1.944	[90]
	oleic acid ethyl ester	5	1.030	1.165-1.491	0.805-1.459	[90]
	oleic acid methyl ester	21	1.029-1.030	1.084-2.168	0.594-1.700	[90,98,104]
	palladium(II) acetylacetonate	125	1.013-1.128	1.152-5.420	1.202-2.076	[79]
	palmitic acid ethyl ester	17	1.013-1.046	1.310-2.852	1.280-1.814	[105]
	n-pentane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	2-pentanone	23	1.013-1.034	1.203-3.963	1.184-1.934	[35]
	3-pentanone	46	1.013-1.079	1.172-4.684	1.261-2.029	[35,82]
	2,4-dimethyl-3-pentanone	8	1.033-1.033	1.355-2.439	1.297-1.738	[39]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	2,2,4,4-tetramethyl-3-pentanone	9	1.031	1.355-2.168	1.330-1.694	[82]
	n-pentylbenzene	31	1.013-1.309	2.033-4.743	1.296-2.034	[63]
	phenanthrene	25	0.997-1.096	1.308-3.734	1.082-1.956	[34,38,95]
	phenol	109	1.013-1.079	1.089-4.103	0.757-1.987	[36,68,72,73]
	phenylacetic acid	16	1.013-1.046	1.310-2.852	1.280-1.814	[106]
	phenylacetylene	15	1.030-1.096	2.033-4.743	1.295-1.997	[85]
	phenylbutazone	78	1.013-1.128	1.152-5.420	0.951-2.074	[107]
	1-phenyldodecane	15	1.029-1.095	2.033-4.743	1.295-1.997	[63]
	1-phenylethanol	15	1.030-1.096	2.033-4.743	1.296-1.998	[108]
	2-phenylethanol	15	1.030-1.096	2.033-4.743	1.296-1.998	[108]
	2-phenylethyl acetate	15	1.030-1.096	2.033-4.743	1.295-1.997	[58]
	1-phenylhexane	15	1.029-1.095	2.033-4.743	1.295-1.997	[63]
	phenylmethanol	15	1.030-1.096	2.033-4.743	1.296-1.998	[108]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	1-phenyloctane	15	1.029-1.095	2.033-4.743	1.295-1.997	[63]
	3-phenylpropyl acetate	15	1.030-1.096	2.033-4.743	1.295-1.997	[58]
	α-pinene	30	1.030-1.096	1.626-3.726	0.953-1.912	[109,110]
	β-pinene	15	1.030-1.096	1.626-2.710	0.953-1.799	[109]
	platinum(II) acetylacetonate	62	1.013-1.128	1.153-5.420	0.954-2.076	[111]
	1-propanol	17	1.030	1.287-2.168	1.236-1.697	[56]
	2-phenyl-1-propanol	15	1.030-1.096	2.033-4.743	1.296-1.998	[108]
	2-propanol	18	1.030	1.287-2.304	1.236-1.725	[56]
	3-phenyl-1-propanol	15	1.030-1.096	2.033-4.743	1.296-1.998	[108]
	i-propylbenzene	36	1.030-1.096	1.762-4.743	1.082-1.996	[34,50,62,112]
	n-propylbenzene	60	1.013-1.096	1.152-4.743	0.764-1.997	[49,50,62,112]
	pyrene	21	0.997-1.096	1.558-47.425	0.832-1.989	[34,44]
	squalene	5	1.034-1.034	1.762-2.439	1.562-1.734	[39]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	stearic acid	4	1.031	1.762-2.168	1.581-1.693	[39]
	stearic acid ethyl ester	17	1.013-1.046	1.310-2.852	1.280-1.814	[47]
	styrene	15	1.030-1.096	2.033-4.743	1.296-1.910	[42]
	n-tetradecane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	tetrahydrofuran	15	1.030-1.096	1.084-2.168	0.418-1.704	[84]
	thenoyltrifluoroacetone	15	1.013-1.046	1.430-3.037	1.210-1.887	[80]
	α-tocopherol	82	1.013-1.096	1.153-4.107	1.311-1.987	[71–73]
	toluene	41	1.007-1.096	1.018-4.743	0.457-1.997	[50,53,68]
	triarachidonin	27	1.030	1.348-4.098	1.333-1.945	[113]
	trierucin	101	1.013-1.063	1.119-4.073	1.204-1.984	[113]
	trifluoroacetylacetone	15	1.013-1.046	1.449-2.924	1.237-1.873	[80]
	1,3,5-trimethylbenzene	34	0.997-1.096	1.287-4.743	1.240-1.996	[34,42,49,61]
	trinervonin	38	1.013-1.063	1.220-4.072	1.268-1.984	[113]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	triolein	14	0.980-1.030	1.237-3.401	1.101-2.015	[13,113]
	ubiquinone CoQ10	80	1.013-1.096	1.153-4.095	1.311-1.984	[73,114]
	n-undecane	5	0.984-1.013	1.220-1.423	1.559-1.745	[83]
	6-undecanone	13	1.034-1.034	1.355-2.439	1.282-1.734	[39]
	vanillin	15	1.013-1.046	1.396-2.852	1.280-1.814	[106]
	vitamin K1	17	1.030	1.355-4.065	1.342-1.943	[81,102]
	vitamin K3	22	1.030	1.214-4.068	1.018-1.943	[73,99,102]
	water	24	0.931-1.013	1.789-4.038	1.695-2.176	[115]
	5-*tert*-butyl-*m*-xylene	31	1.013-1.309	2.033-4.743	1.292-2.033	[85]
	m-xylene	12	1.030-1.227	1.355-4.065	0.403-1.943	[96]
	p-xylene	7	1.030-1.063	2.033-3.388	1.496-1.878	[61,62]
cyclohexane	acetone	4	0.548-0.602	3.931	2.767-2.862	[116]
	argon	7	0.539-0.751	-	2.386-2.833	[117]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	benzene	12	0.539-0.945	3.931; sat.p[a]	1.757-2.862	[116,118]
	carbon tetrachloride	7	0.539-0.751	-	2.386-2.833	[117]
	1,1′-dimethylferrocene	5	0.566-0.584	0.047-4.673	2.780-2.841	[119]
	ethane	5	0.507-0.656	-	2.595-2.906	[120]
	ethylene	5	0.507-0.656	-	2.595-2.906	[120]
	ethylferrocene	6	0.566-0.584	0.042-4.673	2.780-2.841	[119]
	ferrocene	5	0.566-0.584	0.047-4.673	2.780-2.841	[119]
	krypton	6	0.566-0.751	-	2.386-2.781	[117]
	methane	6	0.566-0.751	-	2.386-2.781	[117]
	naphthalene	12	0.539-0.945	3.931; sat.p[a]	1.757-2.862	[116,118]
	phenanthrene	8	0.539-0.945	sat.p[a]	1.757-2.833	[118]
	tetrabutyltin	7	0.539-0.751	-	2.386-2.833	[117]
	tetraethyltin	7	0.539-0.751	-	2.386-2.833	[117]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	tetramethyltin	7	0.539-0.751	-	2.386-2.833	[117]
	tetrapropyltin	6	0.539-0.751	-	2.386-2.833	[117]
	toluene	12	0.539-0.945	3.931; sat.p°	1.757-2.862	[116,118]
	1,3,5-trimethylbenzene	12	0.539-0.945	3.931; sat.p[a]	1.757-2.862	[116,121]
	xenon	7	0.539-0.751	-	2.386-2.833	[117]
	m-xylene	4	0.548-0.602	3.931	2.767-2.862	[116]
	p-xylene	8	0.539-0.945	sat.p[a]	1.757-2.833	[118]
n-decane	argon	3	0.482-0.701	0.047	2.614-3.079	[122]
	carbon tetrachloride	3	0.482-0.604	0.047	2.829-3.079	[122]
	12-crown-4	4	0.483-0.604	0.047	2.829-3.079	[123]
	15-crown-5	4	0.483-0.604	0.047	2.829-3.079	[123]
	18-crown-6	4	0.483-0.604	0.047	2.829-3.079	[123]
	dicyclohexano-18-crown-6	4	0.483-0.604	0.047	2.829-3.079	[123]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	dicyclohexan*o*-24-crown-8	4	0.483-0.604	0.047	2.829-3.079	[123]
	krypton	3	0.482-0.701	0.047	2.614-3.079	[122]
	tetrabutyltin	4	0.482-0.701	0.047	2.614-3.079	[122]
	tetraethyltin	4	0.482-0.701	0.047	2.614-3.079	[122]
	tetramethyltin	4	0.482-0.701	0.047	2.614-3.079	[122]
	tetrapropyltin	4	0.482-0.701	0.047	2.614-3.079	[122]
	s-trioxane	4	0.483-0.604	0.047	2.829-3.079	[123]
	xenon	8	0.458-0.701	0.047	2.614-3.128	[122,124]
2;3-dimethylbutane	benzene	11	1.046-1.096	1.710-5.080	1.432-1.908	[125]
	naphthalene	9	1.046-1.096	1.710-5.080	1.432-1.908	[125]
	phenanthrene	11	1.046-1.096	1.710-5.080	1.432-1.908	[125]
	toluene	10	1.046-1.096	2.005-5.080	1.432-1.908	[125]
n-dodecane	acetone	5	0.461-0.521	8.791	3.040-3.153	[116]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	benzene	4	0.461-0.506	8.791	3.068-3.153	[116]
	carbon dioxide	9	0.462-0.862	0.765-1.898	2.165-3.107	[126]
	carbon monoxide	9	0.462-0.862	0.765-1.898	2.165-3.107	[126]
	n-decane	5	0.462-0.860	0.776-0.796	2.190-3.107	[127]
	n-hexadecane	5	0.462-0.860	0.776-0.796	2.190-3.107	[127]
	linoleic acid methyl ester	4	0.461-0.506	8.791	3.068-3.153	[116]
	naphthalene	5	0.461-0.521	8.791	3.040-3.153	[116]
	n-octane	9	0.462-0.860	0.776-1.890	2.190-3.107	[127]
	n-tetradecane	5	0.462-0.860	0.776-0.796	2.190-3.107	[127]
	toluene	4	0.461-0.506	8.791	3.068-3.153	[116]
	1,3,5-trimethylbenzene	4	0.461-0.506	8.791	3.068-3.153	[116]
	vitamin K3	4	0.461-0.506	8.791	3.068-3.152	[116]
	m-xylene	4	0.461-0.506	8.791	3.068-3.153	[116]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
n-eicosane	carbon dioxide	5	0.488-0.696	1.226	2.685-3.153	[128]
	carbon monoxide	5	0.488-0.696	1.226	2.685-3.153	[128]
	n-dodecane	5	0.489-0.696	1.226	2.685-3.153	[128]
	n-hexadecane	5	0.489-0.696	1.226	2.685-3.153	[128]
	n-octane	5	0.489-0.696	1.226	2.685-3.153	[128]
ethane	1-octene	6	0.970-1.055	1.449-2.295	1.521-1.968	[129]
	1-tetradecene	9	0.960-1.055	1.414-2.295	1.519-1.992	[129]
n-heptane	benzene	11	0.561-0.617	0.036	2.800-2.911	[130,131]
	n-decane	6	0.552-0.883	0.036-1.270	2.182-2.930	[127,132]
	n-dodecane	6	0.552-0.883	0.036-1.296	2.182-2.941	[127,132]
	ethylbenzene	4	0.561-0.617	0.036	2.800-2.911	[131]
	n-hexadecane	9	0.552-0.883	0.036-1.270	2.125-2.930	[127,133]
	n-hexane	11	0.524-0.616	0.036	2.800-2.985	[134–136]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	n-octane	13	0.542-0.883	0.036-1.270	2.182-2.949	[127,134,137]
	n-tetradecane	6	0.552-0.883	0.036-1.296	2.182-2.941	[127,132]
	toluene	4	0.561-0.617	0.036	2.800-2.911	[131]
	1,3,5-trimethylbenzene	4	0.561-0.617	0.036	2.800-2.911	[131]
	2,2,4-trimethylpentane	4	0.570-0.598	0.036	2.838-2.893	[137]
	o-xylene	4	0.561-0.617	0.036	2.800-2.911	[131]
	p-xylene	4	0.561-0.617	0.036	2.800-2.911	[131]
n-hexadecane	carbon dioxide	10	0.448-0.781	0.991-2.454	2.305-3.103	[126]
	carbon monoxide	10	0.448-0.781	0.991-2.454	2.305-3.103	[126]
	n-decane	5	0.448-0.781	1.004-1.021	2.361-3.092	[138]
	n-dodecane	5	0.448-0.781	1.004-1.021	2.361-3.092	[138]
	n-octane	10	0.448-0.781	1.004-2.486	2.361-3.095	[138]
	n-tetradecane	5	0.448-0.781	1.004-1.021	2.361-3.092	[138]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
n-hexane	acetone	5	0.597-0.657	5.316-8.306	2.766-2.873	[116]
	acetonitrile	7	0.588-0.588	0.034-128.106	2.820-3.477	[139]
	benzene	48	0.420-1.070	b	1.352-3.458	[116,120,121,139–143]
	carbon disulfide	10	0.588-0.588	0.034-127.575	2.820-3.476	[139]
	carbon tetrabromide	8	0.587-0.587	0.033-116.279	2.825-3.457	[144]
	o-difluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]
	p-difluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]
	9,10-dimethylanthracene	8	0.587-0.587	0.033-116.279	2.825-3.457	[144]
	1,1′-dimethylferrocene	4	0.617	0.056-6.319	2.759-2.850	[119]
	ethylferrocene	4	0.617	0.053-6.316	2.759-2.850	[119]
	ferrocene	4	0.617	0.056-6.319	2.759-2.850	[119];
	n-heptane	11	0.558-0.784	0.033	2.705-2.883	[134–136,145]
	hexafluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	indole	2	0.617	5.316-8.306	2.833-2.871	[116]
	linoleic acid methyl ester	2	0.617	5.316-8.306	2.833-2.871	[116]
	naphthalene	21	0.587-1.070	c	1.352-2.871	[116,121,139,140]
	octafluorotoluene	7	0.420-0.657	0.033	2.676-3.144	[143]
	n-octane	7	0.581-0.646	0.033	2.705-2.837	[134,145]
	pentafluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]
	phenanthrene	15	0.657-1.070	sat.p[b]; P_r>1	1.352-2.678	[121]
	pyrene	8	0.587-0.587	0.033-116.279	2.825-3.457	[140,144]
	1,2,3,5-tetrafluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]
	1,2,4,5-tetrafluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]
	toluene	32	0.587-1.070	d	1.352-3.468	[116,121,146,147]
	1,2,4-trifluorobenzene	7	0.420-0.657	0.033	2.676-3.144	[143]
	1,3,5-trimethylbenzene	20	0.597-1.070	c	1.352-2.871	[116,121]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	vitamin K3	5	0.617	5.316-8.306	2.837-2.873	[99,116]
	m-xylene	5	0.597-0.657	5.316-8.306	2.766-2.873	[116]
	p-xylene	17	0.617-1.070	c	1.352-2.871	[116,121]
n-octane	argon	4	0.524-0.709	0.040	2.594-3.008	[122]
	benzene	8	0.533-0.586	0.040	2.884-2.990	[131,148]
	carbon tetrachloride	4	0.524-0.656	0.040	2.738-3.008	[122]
	ethylbenzene	8	0.533-0.586	0.040	2.884-2.990	[131,148]
	n-heptane	7	0.515-0.603	0.040	2.849-3.025	[134,149];
	n-hexane	6	0.519-0.585	0.040	2.885-3.018	[134]
	krypton	4	0.524-0.709	0.040	2.594-3.008	[122]
	methane	4	0.524-0.709	0.040	2.594-3.008	[122]
	tetrabutyltin	4	0.524-0.761	0.040	2.498-3.008	[122]
	tetraethyltin	5	0.524-0.761	0.040	2.498-3.008	[122]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	tetramethyltin	4	0.524-0.761	0.040	2.498-3.008	[122]
	tetrapropyltin	4	0.524-0.761	0.040	2.498-3.008	[122]
	toluene	8	0.533-0.586	0.040	2.884-2.990	[131,148]
	1,3,5-trimethylbenzene	8	0.533-0.586	0.040	2.884-2.990	[131,148]
	xenon	8	0.498-0.709	0.040	2.594-3.059	[122,124]
	o-xylene	8	0.533-0.586	0.040	2.884-2.990	[131,148]
	p-xylene	8	0.533-0.586	0.040	2.884-2.990	[131,148]
propane	1-octene	8	0.802-0.913	1.308-2.198	2.030-2.373	[129]
	1-tetradecene	8	0.791-0.912	2.092-2.165	2.103-2.396	[129]
sulfur hexafluoride	benzene	9	1.029-1.029	0.931-3.816	0.408-1.903	[150]
	benzoic acid	6	1.030-1.061	1.729-3.191	1.247-1.904	[105]
	carbon tetrachloride	7	1.029-1.029	0.021-1.920	0.408-1.903	[150]
	naphthalene	5	0.998-1.030	1.729-3.191	1.507-2.025	[105]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	toluene	11	1.029-1.029	0.931-3.816	0.408-1.903	[150]
	1,3,5-trimethylbenzene	10	1.029-1.029	1.117-3.816	0.680-1.903	[150]
	p-xylene	52	0.889-1.061	0.798-3.989	0.408-2.243	[150]
n-tetradecane	acridine	8	0.481-0.683	0.069	2.666-3.079	[151]
	argon	4	0.430-0.620	0.069	2.803-3.171	[122]
	benzothiophene	7	0.481-0.654	0.069	2.731-3.079	[151]
	carbon tetrachloride	4	0.430-0.540	0.069	2.967-3.171	[122]
	dibenzothiophene	8	0.481-0.668	0.069	2.699-3.079	[151]
	krypton	4	0.430-0.620	0.069	2.803-3.171	[122]
	methane	4	0.430-0.620	0.069	2.803-3.171	[122]
	naphthalene	7	0.452-0.654	0.069	2.731-3.132	[151]
	tetrabutyltin	4	0.430-0.620	0.069	2.803-3.171	[122]
	tetraethyltin	4	0.430-0.620	0.069	2.803-3.171	[122]

Solvent	Solute	NDP	T_r	P_r	ρ_r	Source
	tetramethyltin	4	0.430-0.620	0.069	2.803-3.171	[122]
	tetrapropyltin	4	0.430-0.620	0.069	2.803-3.171	[122]
	xenon	8	0.409-0.620	0.069	2.803-3.209	[122,124]
2,2,4-trimethylpentane	benzene	4	0.558-0.613	0.039	2.135-2.216	[148]
	1,3,5-trimethylbenzene	4	0.558-0.613	0.039	2.135-2.216	[148]
	ethylbenzene	4	0.558-0.613	0.039	2.135-2.216	[148]
	toluene	4	0.558-0.613	0.039	2.135-2.216	[148]
	o-xylene	4	0.558-0.613	0.039	2.135-2.216	[148]
	p-xylene	4	0.558-0.613	0.039	2.135-2.216	[148]

262 [a] sat.p.: saturation pressure; [b] P_r from 0.034 to 122.69 and at saturation pressure; [c] P_r=0.498 and 0.532, at saturation pressure and other points at P_r>1; [d] P_r from 0.034 to 124.58 and

263 saturation pressure.

Table A2 – Pure component data, compound name, chemical formula, CAS number, molecular weight,M, critical temperature, T_c, pressure, P_c, and volume, V_c, Lennard-Jones diameter, σ_{LJ}, and energy, ε_{LJ}/k_B.

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
acetone	C_3H_6O	67-64-1	58.08	508.10[a]	47.00[a]	209.00[a]	4.67012[p]	332.97[p]
acetonitrile	C_2H_3N	75-05-8	41.05	545.50[a]	48.30[a]	173.00[a]	4.02424[p]	652.53[p]
acridine	$C_{13}H_9N$	260-94-6	179.22	905.00[b]	36.40[b]	543.00[b]	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]	6.34300[p]	587.58[p]
allylbenzene	C_9H_{10}	300-57-2	118.18	639.86[d]	33.50[d]	419.80[d]	5.91809[p]	495.25[p]
aluminum acetylacetonate	$Al(C_5H_7O_2)_3$	13963-57-0	324.31	437.66[c]	19.57[c]	881.69[c]	6.20646[p]	338.75[p]
aniline	C_6H_7N	62-53-3	93.13	699.00[a]	53.10[a]	274.00[a]	5.27450[p]	541.03[p]
anisole	C_7H_8O	100-66-3	108.14	641.65[l]	41.75[l]	337.00[l]	5.53560[p]	496.64[p]
anthracene	$C_{14}H_{10}$	120-12-7	178.23	873.00[l]	29.00[l]	554.00[l]	6.77034[p]	675.70[p]
arachidonic acid (AA)	$C_{20}H_{32}O_2$	506-32-1	304.47	1013.42[e]	12.74[e]	1093.20[e]	8.55861[p]	784.39[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
AA ethyl ester	$C_{22}H_{36}O_2$	1808-26-0	332.53	960.63[f]	11.31[f]	1195.26[f]	8.64877[p]	743.53[p]
argon	Ar	7440-37-1	39.95	150.80[a]	48.70[a]	74.90[a]	3.40744[p]	123.55[p]
behenic acid ethyl ester	$C_{24}H_{48}O_2$	5908-87-2	368.64	984.94[f]	9.15[f]	1394.66[f]	9.03867[p]	762.34[p]
benzene	C_6H_6	71-43-2	78.11	562.20[a]	48.90[a]	259.00[a]	5.19165[p]	308.43[p]
benzoic acid	$C_7H_6O_2$	65-85-0	122.12	752.00[a]	45.60[a]	341.00[a]	5.65763[p]	582.05[p]
benzothiophene	C_8H_6S	95-15-8	134.2	764.00[g]	47.60[g]	379.00[g]	5.61049[p]	591.34[p]
benzyl acetate	$C_9H_{10}O_2$	140-11-4	150.18	699.00[l]	31.80[l]	449.00[l]	6.17454[p]	541.03[p]
benzylacetone	$C_{10}H_{12}O$	2550-26-7	148.2	722.51[d]	31.20[d]	500.50[d]	6.27139[p]	559.22[p]
biphenyl	$C_{12}H_{10}$	92-52-4	154.21	789.00[a]	38.50[a]	502.00[a]	6.04576[p]	610.69[p]
2-bromoanisole	C_7H_7BrO	578-57-4	187.04	737.58[d]	40.04[d]	378.05[d]	5.85312[p]	570.89[p]
bromobenzene	C_6H_5Br	108-86-1	157.01	670.00[a]	45.20[a]	324.00[a]	5.47376[p]	518.58[p]
2-butanone	C_4H_8O	78-93-3	72.11	536.80[a]	42.10[a]	267.00[a]	5.22195[p]	415.48[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
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]	7.55769[p]	744.64[p]
n-butylbenzene	$C_{10}H_{14}$	104-51-8	134.22	660.50[a]	28.90[a]	497.00[a]	6.24687[p]	511.23[p]
sec-butylbenzene	$C_{10}H_{14}$	135-98-8	134.22	672.06[h]	29.50[h]	478.37[h]	6.24091[p]	520.17[p]
tert-butylbenzene	$C_{10}H_{14}$	98-06-6	134.22	660.00[a]	29.60[l]	492.00[l]	6.20099[p]	510.84[p]
butyric acid ethyl ester	$C_6H_{12}O_2$	105-54-4	116.20	579.00[i]	31.40[i]	400.00[i]	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]	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]	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]	6.82453[p]	507.51[p]
carbon dioxide	CO_2	124-38-9	44.01	304.10[a]	73.80[a]	93.90[a]	3.26192[p]	500.71[p]
carbon disulfide	CS_2	75-15-0	76.13	552.00[a]	79.00[a]	160.00[a]	4.29901[p]	376.51[p]
carbon monoxide	CO	630-08-0	28.01	132.90[a]	35.00[a]	93.20[a]	3.53562[p]	102.86[p]
carbon tetrabromide	CBr_4	558-13-4	331.63	724.91[l]	96.31[l]	328.50[l]	4.41501[p]	561.08[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
carbon tetrachloride	CCl_4	56-23-5	153.82	556.40[a]	45.60[a]	275.90[a]	5.29240[p]	418.84[p]
β-carotene	$C_{40}H_{56}$	7235-40-7	536.88	1450.76[e]	6.90[e]	1934.95[e]	10.08103[p]	1122.89[p]
L-carvone	$C_{10}H_{14}O$	6485-40-1	150.22	709.40[j]	26.30[j]	504.65[j]	6.55942[p]	549.08[p]
chlorobenzene	C_6H_5Cl	108-90-7	112.56	632.40[a]	45.20[a]	308.00[a]	5.56838[p]	207.50[p]
chromium(III) acetylacetonate	$Cr(acac)_3$	21679-31-2	349.32	858.85[c]	18.92[c]	627.04[c]	5.71650[r]	845.60[r]
chrysene	$C_{18}H_{12}$	218-01-9	228.29	979.00[l]	23.90[l]	690.00[l]	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]	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]	6.73800[s]	499.75[s]
copper(II) trifluoroacetylacetonate	$C_{10}H_8CuF_6O_4$	14324-82-4	369.70	412.85[c]	20.63[c]	441.13[c]	6.00245[p]	319.55[p]
12-crown-4	$C_8H_{16}O_4$	294-93-9	176.21	780.66[e]	33.59[e]	444.75[e]	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]	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]	7.26959[p]	751.17[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
dibenzo-24-crown-8	$C_{24}H_{32}O_8$	14174-09-5	448.51	1396.77[e]	15.80[e]	1174.35[e]	8.69916[p]	1081.10[p]
dicyclohexano-18-crown-6	$C_{20}H_{36}O_6$	16069-36-6	372.5	1177.47[e]	16.24[e]	1002.75[e]	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]	8.62250[p]	1050.83[p]
cycloheptanone	$C_7H_{12}O$	502-42-1	112.17	671.19[c]	36.86[c]	297.87[c]	5.83262[p]	519.50[p]
cyclohexane	C_6H_{12}	110-82-7	84.16	553.50[a]	40.70[a]	308.00[a]	5.73075[p]	224.87[p]
cyclononanone	$C_9H_{16}O$	3350-30-9	140.22	702.10[c]	31.47[c]	380.74[c]	6.20229[p]	543.42[p]
cyclopentanone	C_5H_8O	120-92-3	84.12	626.00[l]	58.50[l]	258.00[l]	4.94075[p]	484.52[p]
n-decane	$C_{10}H_{22}$	124-18-5	142.29	617.70[a]	21.20[a]	603.00[a]	6.71395[p]	434.86[p]
docosahexaenoic acid (DHA)	$C_{22}H_{32}O_2$	6217-54-5	328.49	833.67[e]	12.03[e]	1164.30[e]	8.34392[p]	645.26[p]
DHA ethyl ester	$C_{24}H_{36}O_2$	84494-72-4	356.55	828.45[e]	10.52[e]	1276.40[e]	8.54432[p]	641.22[p]
DHA methyl ester	$C_{23}H_{34}O_2$	2566-90-7	342.52	844.78[e]	11.07[e]	1220.85[e]	8.49793[p]	653.86[p]
dibenzothiophene	$C_{12}H_8S$	132-65-0	184.26	897.00[g]	38.60[g]	512.00[g]	6.27791[p]	694.28[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
dibenzyl ether	$C_{14}H_{14}O$	103-50-4	198.26	777.00[l]	25.60[l]	608.00[l]	6.78621[p]	601.40[p]
1,2-dichlorobenzene	$C_6H_4Cl_2$	95-50-1	147	729.00[a]	41.00[a]	360.00[a]	5.79009[p]	564.25[p]
1,3-dichlorobenzene	$C_6H_4Cl_2$	541-73-1	147	683.95[l]	40.70[l]	351.00[l]	5.69056[p]	529.38[p]
p-dichlorobenzene	$C_6H_4Cl_2$	106-46-7	147	684.75[l]	40.70[l]	351.00[l]	5.69261[p]	530.00[p]
diethyl ether	$C_4H_{10}O$	60-29-7	74.12	466.70[a]	36.40[a]	280.00[a]	5.23105[p]	361.23[p]
1,2-diethylbenzene	$C_{10}H_{14}$	135-01-3	134.22	668.00[l]	28.80[l]	502.00[l]	6.27438[p]	517.03[p]
1,4-diethylbenzene	$C_{10}H_{14}$	105-05-5	134.22	657.96[l]	28.03[l]	497.00[l]	6.29672[p]	509.26[p]
o-difluorobenzene	$C_6H_4F_2$	367-11-3	114.09	554.46[l]	40.67[l]	299.50[l]	5.33270[p]	429.15[p]
p-difluorobenzene	$C_6H_4F_2$	540-36-3	114.09	556.00[l]	44.00[l]	299.50[l]	5.20720[p]	430.34[p]
diisopropyl ether	$C_6H_{14}O$	108-20-3	102.18	500.30[a]	28.80[a]	386.00[a]	5.74891[p]	387.23[p]
2,3-dimethylaniline	$C_8H_{11}N$	87-59-2	121.18	717.00[d]	36.30[d]	400.38[d]	5.97871[p]	554.96[p]
2,6-dimethylaniline	$C_8H_{11}N$	87-62-7	121.18	722.00[m]	42.00[d]	400.38[d]	5.73044[p]	558.83[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
9,10-dimethylanthracene	$C_{16}H_{14}$	781-43-1	206.29	899.22[e]	26.27[e]	724.55[e]	7.01984[p]	696.00[p]
2,3-dimethylbutane	C_6H_{14}	79-29-8	86.18	500.00[a]	31.30[a]	358.00[a]	5.60227[p]	387.00[p]
1,1-dimethylferrocene	$C_{12}H_{14}Fe$	1291-47-0	214.09	514.45[c]	27.41[c]	400.64[c]	5.88660[p]	398.18[p]
2,3-dimethylnaphthalene	$C_{12}H_{12}$	581-40-8	156.23	777.78[l]	30.06[l]	521.50[l]	6.48023[p]	602.00[p]
2,6-dimethylnaphthalene	$C_{12}H_{12}$	581-42-0	156.23	777.00[l]	31.70[l]	520.00[l]	6.37790[p]	601.40[p]
2,7-dimethylnaphthalene	$C_{12}H_{12}$	582-16-1	156.23	778.00[l]	31.70[l]	520.00[l]	6.38032[p]	602.17[p]
2,4-dimethylphenol	$C_8H_{10}O$	105-67-9	122.17	707.60[a]	44.00[l]	390.00[l]	5.61388[p]	547.68[p]
diolein	$C_{39}H_{72}O_5$	2465-32-9	621.99	1025.00[b]	7.92[b]	2150.00[b]	10.44146[p]	793.35[p]
disperse blue 14	$C_{16}H_{14}N_2O_2$	2475-44-7	266	1137.33[k]	27.18[k]	765.50[k]	7.41187[p]	880.29[p]
disperse orange 11	$C_{15}H_{11}NO_2$	82-28-0	237.25	1103.62[k]	31.17[k]	670.00[k]	7.08580[p]	854.20[p]
1,3-divinylbenzene	$C_{10}H_{10}$	108-57-6	130.19	692.00[l]	31.20[l]	440.00[l]	6.19117[p]	535.61[p]
n-dodecane	$C_{12}H_{26}$	112-40-3	170.34	658.20[a]	18.20[a]	713.00[a]	7.00451[p]	672.90[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
n-eicosane	$C_{20}H_{42}$	112-95-8	282.56	767.00[a]	11.10[l]	1190.00[l]	8.33954[p]	593.66[p]
eicosapentaenoic acid (EPA)	$C_{20}H_{30}O_2$	10417-94-4	302.46	1020.90[f]	13.47[f]	1059.15[f]	8.48687[p]	790.18[p]
EPA ethyl ester	$C_{22}H_{34}O_2$	84494-70-2	330.51	968.16[f]	11.67[f]	1173.16[f]	8.61744[p]	749.36[p]
EPA methyl ester	$C_{21}H_{32}O_2$	2734-47-6	316.48	890.55[f]	11.90[f]	1187.03[f]	8.46741[p]	689.29[p]
ethane	C_2H_6	74-84-0	30.07	305.40[a]	48.80[a]	148.30[a]	4.17587[p]	213.99[p]
ethanol	C_2H_6O	64-17-5	46.07	513.90[a]	61.40[a]	167.10[a]	4.23738[p]	1291.41[p]
ethyl acetate	$C_4H_8O_2$	141-78-6	88.11	523.20[a]	38.30[a]	286.00[a]	5.33606[p]	404.96[p]
ethyl benzoate	$C_9H_{10}O_2$	93-89-0	150.18	668.70[a]	23.20[l]	489.00[l]	6.68655[p]	517.57[p]
ethylbenzene	C_8H_{10}	100-41-4	106.17	617.20[a]	36.00[a]	374.00[a]	5.72572[p]	477.71[p]
ethylene	C_2H_4	74-85-1	28.05	282.40[a]	50.40[a]	130.40[a]	4.04838[p]	169.08[p]
ethylferrocene	$C_{12}H_{14}Fe$	1273-89-8	214.08	554.21[c]	27.41[c]	400.64[c]	6.02127[p]	428.96[p]
2-ethyltoluene	C_9H_{12}	611-14-3	120.19	651.00[a]	30.40[a]	460.00[a]	6.12635[p]	503.87[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
3-ethyltoluene	C_9H_{12}	620-14-4	120.19	637.00[a]	28.40[a]	490.00[a]	6.21196[p]	493.04[p]
4-ethyltoluene	C_9H_{12}	622-96-8	120.19	640.00[a]	29.40[a]	470.00[a]	6.15660[p]	495.36[p]
eugenol	$C_{10}H_{12}O_2$	97-53-0	164.2	735.31[d]	33.52[d]	447.23[d]	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]	6.37838[p]	608.57[p]
2-fluoroanisole	C_7H_7FO	321-28-8	126.13	644.81[d]	38.11[d]	328.87[d]	5.70253[p]	499.08[p]
fluorobenzene	C_6H_5F	462-06-6	96.1	560.10[a]	45.50[a]	269.00[a]	5.16448[p]	433.52[p]
3-fluorophenol	C_6H_5FO	372-20-3	112.1	665.54[e]	54.83[e]	339.60[e]	5.14165[p]	515.13[p]
geraniol	$C_{10}H_{18}O$	106-24-1	154.25	688.44[e]	25.78[e]	571.30[e]	6.54030[p]	532.85[p]
n-heptane	C_7H_{16}	142-82-5	100.2	540.30[a]	27.40[a]	432.00[a]	5.94356[p]	404.05[p]
2-heptanone	$C_7H_{14}O$	110-43-0	114.19	611.50[a]	34.40[l]	421.00[l]	5.78966[p]	473.30[p]
4-heptanone	$C_7H_{14}O$	123-19-3	114.19	595.31[l]	29.96[l]	433.50[l]	5.98953[p]	460.77[p]
hexachlorobenzene	C_6Cl_6	118-74-1	284.78	825.00[l]	28.50[l]	526.00[l]	6.69481[p]	638.55[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
n-hexadecane	$C_{16}H_{34}$	544-76-3	226.45	722.00[a]	14.10[a]	930.00[a]	7.36480[p]	1669.19[p]
1-hexadecene	$C_{16}H_{32}$	629-73-2	224.43	722.00[g]	14.80[g]	933.00[g]	7.70891[p]	558.83[p]
1,1,1,5,5,5-hexafluoroacetylacetone	$C_5H_2F_6O_2$	1552-22-1	208.06	569.07[f]	27.17[f]	406.05[f]	6.08561[p]	440.46[p]
hexafluorobenzene	C_6F_6	392-56-3	186.06	516.70[a]	33.00[a]	335.00[a]	5.56763[p]	399.93[p]
n-hexane	C_6H_{14}	110-54-3	86.18	507.50[a]	30.10[a]	370.00[a]	5.61841[p]	434.76[p]
ibuprofen	$C_{13}H_{18}O_2$	15687-27-1	206.29	769.63[e]	22.85[e]	686.35[e]	6.98841[p]	595.69 [p]
indole	C_8H_7N	204-420-7	117.15	790.00[l].	43.40[l]	431.00[l]	5.83184 [p]	611.46 [p]
iodobenzene	C_6H_5I	591-50-4	204.01	721.00[a]	45.20[a]	351.00[a]	5.59976[p]	558.05[p]
isobutylbenzene	$C_{10}H_{14}$	538-93-2	134.22	650.00[h]	30.50[h]	480.00[h]	6.11748[p]	503.10[p]
krypton	Kr	7439-90-9	83.8	209.40[a]	55.00[a]	91.20[a]	2.89870[p]	511.92[p]
D-limonene	$C_{10}H_{16}$	5989-27-5	136.24	660.00[l]	27.50[l]	524.00[l]	6.33828[p]	510.84[p]
linalool	$C_{10}H_{18}O$	78-70-6	154.25	645.80[e]	25.95[e]	558.00[e]	6.40654[p]	499.85[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
linoleic acid	$C_{18}H_{32}O_2$	60-33-3	280.45	775.00[b]	14.10[b]	990.00[b]	7.93427[p]	599.85[p]
linoleic acid methyl ester	$C_{19}H_{34}O_2$	112-63-0	294.48	870.78[f]	12.54[f]	1070.95[f]	8.34769[p]	673.98[p]
α-Linolenic acid	$C_{18}H_{30}O_2$	463-40-1	278.44	780.00[b]	14.40[b]	1070.00[b]	7.90702[p]	603.72[p]
γ-linolenic acid	$C_{18}H_{30}O_2$	506-26-3	278.44	958.98[f]	14.17[f]	992.35[f]	8.30482[p]	742.25[p]
γ-linolenic acid ethyl ester	$C_{20}H_{34}O_2$	31450-14-3	306.48	937.01[c]	17.56[c]	797.37[c]	7.87896[p]	725.25[p]
γ-linolenic acid methyl ester	$C_{19}H_{32}O_2$	16326-32-2	292.46	882.79[f]	12.92[f]	1050.86[f]	8.32085[p]	683.28[p]
L-menthone	$C_{10}H_{18}O$	14073-97-3	154.25	699.44[j]	25.30[j]	525.24[j]	6.60650[p]	541.37[p]
methane	CH_4	74-82-8	16.04	190.40[a]	46.00[a]	99.20[a]	3.58484[p]	167.15[p]
methanol	CH_4O	67-56-1	32.04	512.60[a]	80.90[a]	118.00[a]	3.79957[p]	685.96[p]
2-methylanisole	$C_8H_{10}O$	578-58-5	122.17	648.79[d]	35.60[d]	371.70[d]	5.83396[p]	502.16[p]
4-methylanisole	$C_8H_{10}O$	104-93-8	122.17	655.36[d]	35.60[d]	371.70[d]	5.85195[p]	507.25[p]
3-methylbutylbenzene	$C_{11}H_{15}$	2049-94-7	148.25	672.06[h]	26.50[h]	542.47[h]	6.44224[p]	520.17[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
1-methylnaphthalene	$C_{11}H_{10}$	90-12-0	142.2	772.00[g]	36.00[g]	465.00[g]	6.12893[p]	597.53[p]
monoolein	$C_{21}H_{40}O_4$	111-03-5	356.55	885.00[b]	12.40[b]	1210.00[b]	8.39247[p]	684.99[p]
myristic acid ethyl ester	$C_{16}H_{32}O_2$	124-06-1	256.43	789.35[f]	13.89[f]	950.66[f]	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]	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]	7.79244[p]	602.01[p]
naphthalene	$C_{10}H_8$	91-20-3	128.17	748.40[a]	40.50[a]	413.00[a]	5.85874[p]	579.26[p]
1-naphthol	$C_{10}H_8O$	90-15-3	144.17	802.00[l]	47.37[l]	375.50[l]	5.70365[p]	620.75[p]
2-naphthol	$C_{10}H_8O$	135-19-3	144.17	811.40[i]	47.40[i]	375.50[i]	5.72302[p]	628.02[p]
2-nitroanisole	$C_7H_7NO_3$	91-23-6	153.14	782.00[l]	37.60[l]	422.00[l]	6.07271[p]	605.27[p]
nitrobenzene	$C_6H_5NO_2$	98-95-3	123.11	719.00[l]	44.00[l]	349.00[l]	5.64167[p]	556.51[p]
3-nitrotoluene	$C_7H_7NO_2$	99-08-1	137.14	734.00[l]	38.00[l]	441.00[l]	5.93831[p]	568.12[p]
n-nonane	C_9H_{20}	111-84-2	128.26	594.60[a]	22.90[a]	548.00[a]	6.43057[p]	497.35[p]

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			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
2-nonanone	$C_9H_{18}O$	821-55-6	142.24	644.29[l]	24.53[l]	545.50[l]	6.50874[p]	498.68[p]
5-nonanone	$C_9H_{18}O$	502-56-7	142.24	640.00[b]	23.20[b]	560.00[b]	6.60236[p]	495.36[p]
octafluorotoluene	C_7F_8	434-64-0	236.06	534.47[m]	27.05[m]	428.00[m]	5.97931[p]	413.68[p]
n-octane	C_8H_{18}	111-65-9	114.23	568.80[a]	24.90[a]	492.00[a]	6.17328[p]	478.32[p]
1-octene	C_8H_{16}	111-66-0	112.22	566.70[a]	26.20[a]	464.00[a]	6.14478[p]	438.63[p]
oleic acid	$C_{18}H_{34}O_2$	112-80-1	282.47	781.00[b]	13.90[b]	1000.00[b]	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]	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]	8.41384[p]	672.34[p]
palladium(II) acetylacetonate	$C_{10}H_{14}O_4Pd$	14024-61-4	304.64	651.12[c]	4.13[c]	435.41[c]	4.90200[s]	994.14[s]
palmitic acid ethyl ester	$C_{18}H_{36}O_2$	628-97-7	284.48	835.62[f]	12.36[f]	1061.66[f]	8.30307[p]	646.77[p]
pentafluorobenzene	C_6HF_5	363-72-4	168.07	530.97[m]	35.31[m]	324.00[m]	5.49825[p]	410.97[p]
n-pentane	C_5H_{12}	109-66-0	72.15	469.70[a]	33.70[a]	304.00[a]	5.36967[p]	363.55[p]

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			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
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]	6.06486[p]	485.44[p]
2,4-dimethyl-3-pentanone	$C_7H_{14}O$	565-80-0	114.19	576.00[b]	30.20[b]	416.00[b]	5.91550[p]	445.82[p]
2-pentanone	$C_5H_{10}O$	107-87-9	86.13	561.10[a]	36.90[a]	301.00[a]	5.51733[p]	434.29[p]
3-pentanone	$C_5H_{10}O$	96-22-0	86.13	561.00[a]	37.30[a]	336.00[a]	5.49858[p]	434.21[p]
n-pentylbenzene	$C_{11}H_{16}$	538-68-1	148.25	679.90[l]	26.04[l]	550.00[l]	6.49745[p]	526.24[p]
phenanthrene	$C_{14}H_{10}$	85-01-8	178.23	873.00[a]	29.00[a]	554.00[a]	6.77034[p]	675.70[p]
phenol	C_6H_6O	108-95-2	94.11	694.20[a]	61.30[a]	229.00[a]	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]	6.03311[p]	606.47[p]
phenylacetylene	C_8H_6	536-74-3	102.14	655.43[l]	44.03[l]	337.50[l]	5.48099[p]	507.30[p]
phenylbutazone	$C_{19}H_{20}N_2O_2$	50-33-9	308.38	861.18[e]	18.38[e]	933.55[e]	7.63140[p]	666.55[p]
1-phenyldodecane	$C_{18}H_{30}$	123-01-3	246.44	774.26[l]	15.79[l]	1000.00[l]	7.71873[p]	599.28[p]
1-phenylethanol	$C_8H_{10}O$	98-85-1	122.17	675.30[d]	40.60[k*]	392.15[k*]	5.67259[p]	522.68[p]

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			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
2-phenylethanol	$C_8H_{10}O$	60-12-8	122.17	684.00[l]	39.20[l]	387.00[l]	5.75677[p]	529.42[p]
2-phenylethyl acetate	$C_{10}H_{12}O_2$	103-45-7	164.1	712.23[d]	30.12[d]	524.15[d]	6.31046[p]	551.27[p]
1-phenylhexane	$C_{12}H_{18}$	1077-16-3	162.28	698.00[l]	23.80[l]	618.00[l]	6.71996[p]	540.25[p]
phenylmethanol	C_7H_8O	100-51-6	108.14	720.20[a]	44.00[l]	335.00[l]	5.64457[p]	557.43[p]
1-phenyloctane	$C_{14}H_{22}$	2189-60-8	190.33	729.00[l]	20.20[l]	703.00[l]	7.12309[p]	564.25[p]
3-phenylpropyl acetate	$C_{11}H_{14}O_2$	122-72-5	178.3	718.70[d]	27.23[d]	580.37[d]	6.51801[p]	556.27[p]
α-pinene	$C_{10}H_{16}$	80-56-8	136.24	632.00[l]	27.60[l]	504.00[l]	6.25044[p]	489.17[p]
β-pinene	$C_{10}H_{16}$	127-91-3	136.24	643.00[l]	27.60[l]	506.00[l]	6.28262[p]	497.68[p]
platinum(II) acetylacetonate	$Pt(acac)_2$	15170-57-7	393.29	-	-	-	5.22900[s]	975.45[s]
propane	C_3H_8	74-98-6	44.09	369.80[a]	42.50[a]	203.00[a]	4.50412[p]	457.99[p]
1-propanol	C_3H_8O	71-23-8	60.10	536.80[a]	51.70[a]	219.00[a]	4.49190[p]	2120.83[p]
2-phenyl-1-propanol	$C_9H_{12}O$	1123-85-9	136.20	662.02[d]	36.90[d]	443.23[d]	5.80605[p]	512.40[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
2-propanol	C_3H_8O	67-63-0	60.10	508.30[a]	47.60[a]	220.00[a]	4.93749[p]	393.42[p]
3-phenyl-1-propanol	$C_9H_{12}O$	122-97-4	136.2	702.30[d]	36.40[d]	455.45[d]	5.93627[p]	543.58[p]
i-propylbenzene	C_9H_{12}	98-82-8	120.19	631.10[a]	32.10[l]	427.70[l]	5.97029[p]	488.47[p]
n-propylbenzene	C_9H_{12}	103-65-1	120.19	638.20[a]	32.00[a]	440.00[a]	5.99624[p]	493.97[p]
pyrene	$C_{16}H_{10}$	129-00-0	202.25	936.00[l]	26.10[l]	630.00[l]	7.11077[p]	724.46[p]
squalene	$C_{30}H_{50}$	111-02-4	410.73	716.50[n]	7.03[n]	1601.00[k*]	9.46409 [p]	554.57 [p]
stearic acid	$C_{18}H_{36}O_2$	57-11-4	284.48	803.00[g]	13.30[g]	1140.00[g]	8.10600[p]	621.52[p]
stearic acid ethyl ester	$C_{20}H_{40}O_2$	111-61-5	312.53	777.90[g]	10.19[g]	1380.00[g]	8.49783[p]	602.09[p]
styrene	C_8H_8	100-42-5	104.15	647.00[a]	39.90[l]	352.00[l]	5.62827[p]	500.78[p]
sulfur hexafluoride	SF_6	2551-62-4	146.05	318.70[a]	37.60[a]	198.80[a]	4.76629[p]	271.68[p]
tetrabutyltin	$C_{16}H_{36}Sn$	1461-25-2	347.17	767.97[c]	17.25[c]	760.75[c]	7.53290[p]	594.41[p]
n-tetradecane	$C_{14}H_{30}$	629-59-4	198.39	693.00[a]	14.40[a]	830.00[a]	7.68286[p]	536.38[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
1-tetradecene	$C_{14}H_{28}$	1120-36-1	196.37	691.00[g]	16.27[g]	865.00[g]	7.44105[p]	534.83[p]
tetraethyltin	$C_8H_{20}Sn$	597-64-8	234.95	655.92[c]	25.75[c]	429.28[c]	6.45047[p]	507.68[p]
1,2,3,5-tetrafluorobenzene	$C_6H_2F_4$	2367-82-0	150.08	555.49[e]	36.40[e]	351.05[e]	5.52349[p]	429.95[p]
1,2,4,5-tetrafluorobenzene	$C_6H_2F_4$	327-54-8	150.07	535.25[m]	37.47[e]	351.05[e]	5.41106[p]	414.28[p]
tetrahydrofuran	C_4H_8O	109-99-9	72.11	540.10[a]	51.90[a]	224.00[a]	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]	5.49115[p]	396.11[p]
tetrapropyltin	$C_{12}H_{28}Sn$	2176-98-9	291.06	759.88[c]	20.66[c]	595.01[c]	7.16031[p]	588.15[p]
thenoyltrifluoroacetone	$C_8H_5F_3O_2S$	326-91-0	222.18	838.69[c]	26.32[c]	428.15[c]	6.88081[p]	649.15[p]
α-tocopherol	$C_{29}H_{50}O_2$	10191-41-0	430.71	915.76[o]	8.46[o]	1534.20[o]	9.33059[p]	708.80[p]
toluene	C_7H_8	108-88-3	92.140	591.80[a]	41.00[a]	316.00[a]	5.45450[p]	350.74[p]
triarachidonin	$C_{63}H_{98}O_6$	23314-57-0	951.45	1499.66[c]	6.51[c]	2341.53[c]	10.74274[p]	1160.74[p]
trierucin	$C_{69}H_{128}O_6$	2752-99-0	1053.75	1549.28[c]	5.62[c]	2832.93[c]	11.44706[p]	1199.14[p]

Name	Formula	CAS	M	T_c	P_c	V_c	σ_{LJ}	ε_{LJ}/k_B
			g mol^{-1}	K	bar	cm^3 mol^{-1}	Å	K
trifluoroacetylacetone	$C_5H_5F_3O_2$	367-57-7	154.09	594.02[f]	32.89[f]	365.58[f]	5.81789[p]	459.77[p]
1,2,4-trifluorobenzene	$C_6H_3F_3$	367-23-7	132.09	558.22[e]	38.98[e]	335.05[e]	5.41530[p]	432.06[p]
1,3,5-trimethylbenzene	C_9H_{12}	108-67-8	120.19	637.30[a]	31.30[l]	433.00[l]	6.03392[p]	493.27[p]
2,2,4-trimethylpentane	C_8H_{18}	540-84-1	144.23	543.80[l]	25.70[l]	468.00[l]	6.10433[p]	420.90[p]
trinervonin	$C_{75}H_{140}O_6$	81913-24-8	1137.91	1601.10[c]	5.20[c]	3081.54[c]	11.77257[p]	1239.25[p]
triolein	$C_{57}H_{104}O_6$	122-32-7	885.43	1640.00[b]	4.70[b]	3090.00[b]	11.78333[p]	1269.36[p]
s-trioxane	$C_3H_6O_3$	110-88-3	90.08	604.00[l]	58.20[l]	206.00[l]	4.89292[p]	467.50[p]
ubiquinone CoQ10	$C_{59}H_{90}O_4$	303-98-0	863.34	1522.50[c]	7.09[c]	2146.17[c]	10.43527[p]	1178.41[p]
n-undecane	$C_{11}H_{24}$	1120-21-4	156.31	638.80[a]	19.70[a]	660.00[a]	6.91444[p]	494.43[p]
6-undecanone	$C_{11}H_{22}O$	927-49-1	170.30	678.01[b]	20.46[b]	657.50[b]	6.95669[p]	524.78[p]
vanillin	$C_8H_8O_3$	121-33-5	152.15	777.00[l]	40.10[l]	415.00[l]	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]	9.50177[p]	1029.06[p]

Name	Formula	CAS	M g mol^{-1}	T_c K	P_c bar	V_c cm^3 mol^{-1}	σ_{LJ} Å	ε_{LJ}/k_B K
vitamin K3	$C_{11}H_8O_2$	58-27-5	172.18	893.85[e]	31.96[e]	537.20[e]	6.62867[P]	691.84[P]
water	H_2O	7732-18-5	18.02	647.30[a]	221.20[a]	57.10[a]	3.24681[P]	501.01[P]
xenon	Xe	7440-63-3	131.30	289.70[a]	58.40[a]	118.40[a]	3.85754[P]	224.23[P]
5-*tert*-butyl-*m*-xylene	$C_{12}H_{18}$	98-19-1	162.28	684.85[d]	23.90[d]	591.75[d]	6.67527[P]	530.07[P]
m-xylene	C_8H_{10}	108-38-3	106.17	617.10[a]	35.40[a]	376.00[a]	5.75507[P]	477.64[P]
o-xylene	C_8H_{10}	95-47-6	106.17	630.30[a]	37.30[a]	369.00[a]	5.70029[P]	487.85[P]
p-xylene	C_8H_{10}	106-42-3	106.17	616.20[a]	35.10[a]	379.00[a]	5.76754[P]	476.94[P]

[a] taken from Reid *et al* [10];

[b] Taken from Yaws (2008) [152];

[c] Estimated by the Klincewicz method [10,153];

[d] Average of the values by the Joback [10,154,155] and Wen-Qiang [156] methods;

[e] Average of the values by the Joback [10,154,155] and Ambrose [10,157,158] methods;

[f] Average of the values by the Joback [10,154,155] and Somayajulu [159] methods;

[g] Taken from DIPPR database [160] ;

[h] Taken from Pizarro *et al.*[64];

[i] Taken from Table 4 of Liu and Ruckenstein [161];

[j] Average of the values by the Joback [10,154,155] and Constantinou-Gani [162] methods;

[l] Taken from Yaws (1998) [30];

[k] Estimated by the Joback method [10,154,155];

[m] Taken from Korea Thermophysical Properties Data Bank (KDB) [163] ;

[n] Taken from Catchpol *et al* [164];

[o] Taken from ASPEN database [165];

[p] Taken from Silva and Liu 2008 [24];

[q] Estimated by equation (8) and (9) of the manuscript.

[r] Taken from Cordeiro *et al.* [76];

[s] Taken from Cordeiro [166].

286 **Table A3 –** Calculated results obtained by TLSM, TLSM$_d$ and TLSM$_{en}$ models for each individual system: AARD and binary interaction

287 parameters ($k_{12,\mathrm{d}}$ and $k_{12,en}$).

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,\mathrm{d}}$	AARD	$k_{12,\mathrm{en}}$	AARD
carbon dioxide	acetone	213	8.08	3.527×10^{-2}	4.26	1.636×10^{-1}	4.25
	acridine	6	16.10	7.834×10^{-2}	1.95	3.011×10^{-1}	1.97
	adamantanone	8	44.85	2.594×10^{-1}	2.54	8.952×10^{-1}	2.54
	allylbenzene	15	11.65	6.974×10^{-2}	2.99	3.012×10^{-1}	3.08
	aluminum acetylacetonate	84	28.16	-1.021×10^{-1}	10.47	-5.035×10^{-1}	10.40
	aniline	15	7.77	-3.358×10^{-2}	2.98	-1.358×10^{-1}	3.02
	anisole	15	8.94	4.683×10^{-2}	2.06	1.990×10^{-1}	2.08
	anthracene	22	27.81	1.487×10^{-1}	3.88	5.928×10^{-1}	4.02
	arachidonic acid (AA)	75	21.42	1.167×10^{-1}	2.13	4.831×10^{-1}	2.04
	AA ethyl ester	48	24.51	1.329×10^{-1}	2.43	5.597×10^{-1}	2.46

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	behenic acid ethyl ester	17	26.95	1.426×10^{-1}	3.66	5.990×10^{-1}	3.75
	benzene	249	14.49	8.606×10^{-2}	7.38	4.087×10^{-1}	7.39
	benzoic acid	35	15.92	8.952×10^{-2}	5.50	3.435×10^{-1}	5.71
	benzyl acetate	15	10.02	5.357×10^{-2}	2.21	2.230×10^{-1}	2.28
	benzylacetone	15	8.55	4.499×10^{-2}	2.32	1.861×10^{-1}	2.42
	biphenyl	24	19.60	1.084×10^{-1}	3.41	4.144×10^{-1}	3.24
	2-bromoanisole	15	10.73	5.827×10^{-2}	2.37	2.335×10^{-1}	2.49
	bromobenzene	21	17.17	9.406×10^{-2}	4.48	3.849×10^{-1}	4.42
	2-butanone	40	16.69	8.819×10^{-2}	1.91	3.854×10^{-1}	2.02
	N-(4-methoxybenzylidene)-4-*n*-butylaniline	5	43.94	2.537×10^{-1}	1.77	8.798×10^{-1}	1.77
	n-butylbenzene	15	14.55	7.993×10^{-2}	1.90	3.391×10^{-1}	2.06

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	sec-butylbenzene	15	13.24	7.043×10^{-2}	2.14	3.069×10^{-1}	2.15
	tert-butylbenzene	15	15.15	9.035×10^{-2}	3.87	3.935×10^{-1}	4.10
	butyric acid ethyl ester	16	17.21	8.674×10^{-2}	3.64	3.765×10^{-1}	3.73
	caffeine	25	10.86	4.492×10^{-2}	7.92	1.783×10^{-1}	7.93
	capric acid ethyl ester	16	22.35	1.163×10^{-1}	3.85	4.976×10^{-1}	3.95
	caprylic acid ethyl ester	16	19.72	1.049×10^{-1}	2.93	4.529×10^{-1}	3.05
	β-carotene	90	20.78	1.090×10^{-1}	1.38	4.299×10^{-1}	1.56
	L-carvone	27	15.03	8.176×10^{-2}	3.51	3.467×10^{-1}	3.48
	chlorobenzene	21	3.30	5.238×10^{-3}	3.24	2.997×10^{-2}	3.24
	chromium(III) acetylacetonate	104	6.59	-2.393×10^{-2}	5.21	-8.593×10^{-2}	5.14
	chrysene	4	31.87	1.698×10^{-1}	1.45	6.461×10^{-1}	2.03
	citral	15	20.87	1.076×10^{-1}	3.19	4.658×10^{-1}	3.45

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	cobalt(III) acetylacetonate	38	1.58	-4.436×10^{-5}	1.58	-2.065×10^{-4}	1.58
	copper(II) trifluoroacetylacetonate	12	17.80	-8.246×10^{-2}	4.73	-4.225×10^{-1}	4.67
	15-crown-5	29	25.45	1.457×10^{-1}	5.18	5.657×10^{-1}	5.17
	dibenzo-24-crown-8	28	25.90	1.459×10^{-1}	2.06	5.374×10^{-1}	2.19
	cycloheptanone	8	14.56	6.630×10^{-2}	2.95	2.751×10^{-1}	2.95
	cyclononanone	8	14.98	7.446×10^{-2}	3.25	3.097×10^{-1}	3.25
	cyclopentanone	8	3.90	1.799×10^{-2}	1.04	7.338×10^{-2}	1.04
	n-decane	5	41.43	2.252×10^{-1}	3.70	8.614×10^{-1}	3.96
	dibenzyl ether	15	9.54	5.142×10^{-2}	2.14	2.131×10^{-1}	2.25
	1,2-dichlorobenzene	15	16.63	8.500×10^{-2}	1.48	3.478×10^{-1}	1.54
	1,3-dichlorobenzene	4	10.71	4.902×10^{-2}	3.78	2.004×10^{-1}	3.78
	p-dichlorobenzene	13	14.25	6.710×10^{-2}	3.54	2.641×10^{-1}	3.49

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	diethyl ether	17	16.27	2.910×10^{-2}	16.18	1.371×10^{-1}	16.12
	1,2-diethylbenzene	15	14.41	7.676×10^{-2}	1.79	3.326×10^{-1}	1.83
	1,4-diethylbenzene	15	14.13	7.719×10^{-2}	2.98	3.395×10^{-1}	3.12
	diisopropyl ether	15	14.79	3.390×10^{-2}	12.60	1.632×10^{-1}	12.55
	2,3-dimethylaniline	15	4.01	1.764×10^{-2}	1.95	7.548×10^{-2}	1.92
	2,6-dimethylaniline	15	4.62	2.212×10^{-2}	2.66	9.091×10^{-2}	2.67
	1,1′-dimethylferrocene	68	7.83	4.436×10^{-2}	2.78	2.036×10^{-1}	2.77
	2,3-dimethylnaphthalene	3	19.15	1.005×10^{-1}	1.29	4.015×10^{-1}	1.29
	2,6-dimethylnaphthalene	6	17.56	9.741×10^{-2}	3.84	3.876×10^{-1}	3.84
	2,7-dimethylnaphthalene	6	20.15	9.182×10^{-2}	4.35	3.657×10^{-1}	4.35
	2,4-dimethylphenol	15	5.13	2.221×10^{-2}	2.58	8.975×10^{-2}	2.62
	diolein	9	23.51	1.245×10^{-1}	1.64	5.521×10^{-1}	1.64

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	disperse blue 14	47	32.69	1.780×10^{-1}	2.61	6.471×10^{-1}	2.83
	disperse orange 11	65	33.85	1.873×10^{-1}	3.70	6.727×10^{-1}	4.01
	1,3-divinylbenzene	15	17.23	8.848×10^{-2}	1.09	3.760×10^{-1}	1.10
	docosahexaenoic acid (DHA)	63	10.84	5.786×10^{-2}	1.35	2.594×10^{-1}	1.32
	DHA ethyl ester	65	19.78	1.047×10^{-1}	2.28	4.690×10^{-1}	2.36
	DHA methyl ester	17	21.27	1.122×10^{-1}	3.00	4.910×10^{-1}	3.10
	n-dodecane	5	47.19	2.593×10^{-1}	5.39	8.841×10^{-1}	5.73
	eicosapentaenoic acid (EPA)	55	21.19	1.148×10^{-1}	1.20	4.697×10^{-1}	1.13
	EPA ethyl ester	48	25.01	1.339×10^{-1}	2.80	5.607×10^{-1}	2.86
	EPA methyl ester	17	22.87	1.212×10^{-1}	3.62	5.137×10^{-1}	3.68
	ethanol	24	32.30	1.827×10^{-1}	3.00	5.016×10^{-1}	3.00
	ethyl acetate	16	19.23	1.927×10^{-2}	19.00	8.862×10^{-2}	18.96

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	ethyl benzoate	15	16.97	7.818×10^{-2}	4.93	3.526×10^{-1}	5.07
	ethylbenzene	15	17.47	9.140×10^{-2}	2.07	3.936×10^{-1}	2.08
	2-ethyltoluene	15	13.95	7.786×10^{-2}	3.28	3.373×10^{-1}	3.33
	3-ethyltoluene	15	14.42	7.504×10^{-2}	3.59	3.291×10^{-1}	3.64
	4-ethyltoluene	15	11.85	6.179×10^{-2}	2.68	2.766×10^{-1}	2.70
	eugenol	15	4.75	2.181×10^{-2}	3.36	8.958×10^{-2}	3.38
	ferrocene	107	27.63	1.568×10^{-1}	4.35	6.111×10^{-1}	4.43
	2-fluoroanisole	15	7.58	4.079×10^{-2}	1.66	1.749×10^{-1}	1.69
	fluorobenzene	15	5.58	2.650×10^{-2}	3.64	1.173×10^{-1}	3.67
	3-fluorophenol	4	4.04	-2.299×10^{-2}	3.86	-9.190×10^{-2}	3.86
	geraniol	4	4.70	8.590×10^{-3}	3.91	3.678×10^{-2}	3.91
	n-heptane	5	33.05	1.755×10^{-1}	3.31	7.230×10^{-1}	3.55

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	2-heptanone	11	37.88	2.030×10^{-1}	4.47	7.883×10^{-1}	4.47
	4-heptanone	9	44.43	2.517×10^{-1}	2.19	9.004×10^{-1}	2.19
	hexachlorobenzene	14	25.93	1.569×10^{-1}	7.77	6.292×10^{-1}	7.47
	1-hexadecene	11	18.17	8.566×10^{-2}	11.13	3.954×10^{-1}	11.24
	1,1,1,5,5,5-hexafluoroacetylacetone	15	6.66	3.640×10^{-2}	4.08	1.619×10^{-1}	4.07
	n-hexane	5	29.45	1.489×10^{-1}	2.85	6.075×10^{-1}	3.00
	ibuprofen	99	20.40	1.113×10^{-1}	3.05	4.750×10^{-1}	3.24
	iodobenzene	20	14.67	7.925×10^{-2}	2.62	3.173×10^{-1}	2.61
	isobutylbenzene	15	12.54	6.819×10^{-2}	2.35	3.015×10^{-1}	2.43
	D-limonene	15	19.73	1.076×10^{-1}	3.15	4.545×10^{-1}	3.23
	linalool	15	16.58	8.349×10^{-2}	3.49	3.709×10^{-1}	3.51
	linoleic acid	71	12.78	7.314×10^{-2}	3.25	3.221×10^{-1}	3.25

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	linoleic acid methyl ester	20	20.90	1.089×10^{-1}	1.27	4.672×10^{-1}	1.33
	α-Linolenic acid	56	14.47	7.551×10^{-2}	1.83	3.355×10^{-1}	1.93
	γ-linolenic acid	142	21.27	1.154×10^{-1}	2.79	4.849×10^{-1}	2.65
	γ-linolenic acid ethyl ester	41	16.79	9.356×10^{-2}	6.27	4.056×10^{-1}	6.07
	γ-linolenic acid methyl ester	52	21.01	1.104×10^{-1}	5.39	4.782×10^{-1}	5.33
	L-menthone	23	17.77	9.704×10^{-2}	4.05	4.058×10^{-1}	3.97
	methanol	10	14.39	8.571×10^{-2}	3.90	2.931×10^{-1}	3.90
	2-methylanisole	15	8.57	4.704×10^{-2}	1.99	2.002×10^{-1}	1.95
	4-methylanisole	15	3.19	1.435×10^{-2}	2.41	6.308×10^{-2}	2.41
	3-methylbutylbenzene	15	13.79	7.579×10^{-2}	2.61	3.372×10^{-1}	2.64
	1-methylnaphthalene	11	10.04	7.049×10^{-4}	10.02	1.055×10^{-1}	10.01
	monoolein	11	13.91	7.215×10^{-2}	1.40	3.113×10^{-1}	1.40

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	myristic acid ethyl ester	16	23.88	1.322×10^{-1}	3.84	5.586×10^{-1}	3.96
	myristoleic acid	42	16.09	8.700×10^{-2}	4.06	3.888×10^{-1}	3.93
	myristoleic acid methyl ester	81	11.14	4.107×10^{-2}	9.86	1.887×10^{-1}	9.95
	naphthalene	114	19.97	1.206×10^{-1}	9.98	4.706×10^{-1}	9.84
	1-naphthol	11	28.26	1.545×10^{-1}	2.18	5.879×10^{-1}	2.48
	2-naphthol	16	30.20	1.630×10^{-1}	2.53	6.171×10^{-1}	3.02
	2-nitroanisole	15	9.94	5.277×10^{-2}	1.63	2.193×10^{-1}	1.65
	nitrobenzene	23	12.04	6.199×10^{-2}	1.92	2.492×10^{-1}	1.94
	3-nitrotoluene	15	12.84	6.903×10^{-2}	2.74	2.845×10^{-1}	2.87
	n-nonane	5	41.26	2.224×10^{-1}	3.65	8.339×10^{-1}	3.93
	2-nonanone	10	44.20	2.519×10^{-1}	4.21	9.013×10^{-1}	4.21
	5-nonanone	12	42.00	2.331×10^{-1}	4.95	8.695×10^{-1}	4.95

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	n-octane	5	38.36	2.028×10^{-1}	3.65	7.796×10^{-1}	3.83
	oleic acid	19	12.15	7.038×10^{-2}	2.52	3.101×10^{-1}	2.52
	oleic acid ethyl ester	5	11.85	5.355×10^{-2}	5.87	2.332×10^{-1}	5.87
	oleic acid methyl ester	21	10.33	1.934×10^{-2}	9.49	8.476×10^{-2}	9.49
	palladium(II) acetylacetonate	125	2.45	-5.920×10^{-4}	2.45	-2.577×10^{-3}	2.45
	palmitic acid ethyl ester	17	22.88	1.223×10^{-1}	3.18	5.192×10^{-1}	3.24
	n-pentane	5	20.76	9.650×10^{-2}	3.15	4.276×10^{-1}	3.29
	2-pentanone	23	18.45	9.925×10^{-2}	2.06	4.264×10^{-1}	2.09
	3-pentanone	46	17.95	9.521×10^{-2}	2.17	4.154×10^{-1}	2.25
	2,4-dimethyl-3-pentanone	8	4.49	1.518×10^{-2}	3.25	6.728×10^{-2}	3.25
	2,2,4,4-tetramethyl-3-pentanone	9	41.73	2.353×10^{-1}	2.92	8.663×10^{-1}	2.92
	n-pentylbenzene	31	15.12	8.162×10^{-2}	2.04	3.628×10^{-1}	2.58

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	phenanthrene	25	32.75	1.849×10^{-1}	4.88	6.966×10^{-1}	4.90
	phenol	109	13.55	6.924×10^{-2}	3.12	2.720×10^{-1}	3.23
	phenylacetic acid	16	17.71	8.841×10^{-2}	2.01	3.489×10^{-1}	2.10
	phenylacetylene	15	8.67	4.420×10^{-2}	1.22	1.901×10^{-1}	1.20
	phenylbutazone	78	15.46	8.141×10^{-2}	4.25	3.398×10^{-1}	4.56
	1-phenyldodecane	15	5.83	2.986×10^{-2}	2.37	1.310×10^{-1}	2.39
	1-phenylethanol	15	4.81	2.204×10^{-2}	1.84	9.269×10^{-2}	1.90
	2-phenylethanol	15	5.33	2.654×10^{-2}	2.00	1.116×10^{-1}	2.07
	2-phenylethyl acetate	15	4.49	2.439×10^{-2}	2.09	1.042×10^{-1}	2.14
	1-phenylhexane	15	13.96	7.293×10^{-2}	1.95	3.162×10^{-1}	2.03
	phenylmethanol	15	9.56	4.882×10^{-2}	1.79	1.953×10^{-1}	1.80
	1-phenyloctane	15	16.15	8.159×10^{-2}	2.57	3.508×10^{-1}	2.68

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	3-phenylpropyl acetate	15	4.77	2.310×10^{-2}	2.56	9.950×10^{-2}	2.62
	α-pinene	30	14.78	7.001×10^{-2}	3.82	3.091×10^{-1}	3.86
	β-pinene	15	22.55	1.215×10^{-1}	3.59	5.223×10^{-1}	3.80
	platinum(II) acetylacetonate	62	4.53	2.646×10^{-3}	4.52	-8.552×10^{-5}	4.53
	1-propanol	17	42.27	2.413×10^{-1}	4.99	5.578×10^{-1}	4.99
	2-phenyl-1-propanol	15	1.82	3.723×10^{-3}	1.73	1.627×10^{-2}	1.73
	2-propanol	18	12.06	6.693×10^{-2}	3.97	2.929×10^{-1}	3.97
	3-phenyl-1-propanol	15	5.52	2.827×10^{-2}	2.17	1.188×10^{-1}	2.21
	i-propylbenzene	36	17.90	9.507×10^{-2}	2.22	4.068×10^{-1}	2.20
	n-propylbenzene	60	15.56	8.636×10^{-2}	8.20	3.769×10^{-1}	8.23
	pyrene	21	26.97	1.383×10^{-1}	4.78	5.567×10^{-1}	4.78
	squalene	5	28.01	1.546×10^{-1}	4.89	6.983×10^{-1}	4.89

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	stearic acid	4	50.62	2.956×10^{-1}	1.34	9.550×10^{-1}	1.34
	stearic acid ethyl ester	17	20.32	1.116×10^{-1}	3.46	4.993×10^{-1}	3.56
	styrene	15	7.24	3.773×10^{-2}	4.10	1.608×10^{-1}	4.12
	n-tetradecane	5	43.49	2.469×10^{-1}	7.77	8.963×10^{-1}	8.06
	tetrahydrofuran	15	14.86	1.550×10^{-2}	14.70	6.823×10^{-2}	14.67
	thenoyltrifluoroacetone	15	14.93	7.263×10^{-2}	3.09	2.970×10^{-1}	3.01
	α-tocopherol	82	27.71	1.492×10^{-1}	1.36	6.366×10^{-1}	1.69
	toluene	41	15.70	5.181×10^{-2}	11.09	2.528×10^{-1}	11.01
	triarachidonin	27	21.83	1.201×10^{-1}	3.16	4.831×10^{-1}	3.16
	trierucin	101	17.30	9.498×10^{-2}	4.99	4.024×10^{-1}	5.03
	trifluoroacetylacetone	15	17.33	9.123×10^{-2}	1.82	3.893×10^{-1}	1.91
	1,3,5-trimethylbenzene	34	12.15	6.586×10^{-2}	4.31	2.840×10^{-1}	4.34

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	trinervonin	38	18.93	1.023×10^{-1}	4.11	4.299×10^{-1}	4.18
	triolein	14	31.18	1.768×10^{-1}	3.36	6.971×10^{-1}	3.18
	ubiquinone CoQ10	80	20.66	1.042×10^{-1}	2.69	4.122×10^{-1}	2.98
	n-undecane	5	44.60	2.439×10^{-1}	4.47	8.876×10^{-1}	4.76
	6-undecanone	13	43.55	2.432×10^{-1}	4.89	8.882×10^{-1}	4.89
	vanillin	15	11.51	5.834×10^{-2}	1.92	2.292×10^{-1}	1.99
	vitamin K_1	17	34.25	1.915×10^{-1}	2.36	7.209×10^{-1}	2.36
	vitamin K_3	22	26.50	1.491×10^{-1}	3.82	5.699×10^{-1}	3.82
	water	24	27.32	-1.278×10^{-1}	13.05	-4.545×10^{-1}	12.45
	5-*tert*-butyl-*m*-xylene	31	15.30	8.362×10^{-2}	2.26	3.683×10^{-1}	2.55
	m-xylene	12	20.78	1.368×10^{-2}	20.09	6.393×10^{-2}	20.08
	p-xylene	7	18.73	1.067×10^{-1}	3.48	4.485×10^{-1}	3.55

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
cyclohexane	acetone	4	11.30	4.955×10^{-2}	3.09	2.934×10^{-1}	2.91
	argon	7	20.10	1.014×10^{-1}	11.80	6.802×10^{-1}	11.22
	benzene	12	6.29	1.041×10^{-2}	6.07	1.316×10^{-1}	5.79
	carbon tetrachloride	7	12.65	6.568×10^{-2}	3.56	3.747×10^{-1}	2.79
	1,1′-dimethylferrocene	5	4.87	-1.757×10^{-2}	3.07	-9.921×10^{-2}	3.06
	ethane	5	10.47	1.348×10^{-2}	10.21	9.491×10^{-2}	10.09
	ethylene	5	11.37	-8.498×10^{-3}	10.84	-6.578×10^{-2}	10.91
	ethylferrocene	6	1.27	1.273×10^{-3}	1.19	6.962×10^{-3}	1.19
	ferrocene	5	20.25	9.568×10^{-2}	2.90	4.474×10^{-1}	2.98
	krypton	6	17.70	6.549×10^{-2}	10.23	3.981×10^{-1}	9.65
	methane	6	16.61	-9.605×10^{-2}	7.38	-9.052×10^{-1}	8.24
	naphthalene	12	13.89	7.168×10^{-2}	7.66	3.963×10^{-1}	6.07

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	phenanthrene	8	16.34	6.352×10^{-2}	6.30	4.505×10^{-1}	4.70
	tetrabutyltin	7	2.50	1.148×10^{-3}	2.47	5.699×10^{-3}	2.47
	tetraethyltin	7	12.07	5.894×10^{-2}	2.90	3.212×10^{-1}	2.42
	tetramethyltin	7	11.58	6.154×10^{-2}	4.54	3.577×10^{-1}	3.82
	tetrapropyltin	6	9.27	3.977×10^{-2}	3.07	2.710×10^{-1}	2.75
	toluene	12	8.91	4.090×10^{-2}	7.89	2.728×10^{-1}	7.07
	1,3,5-trimethylbenzene	12	8.44	4.280×10^{-2}	6.81	2.356×10^{-1}	5.90
	xenon	7	19.53	9.196×10^{-2}	10.48	5.855×10^{-1}	9.74
	m-xylene	4	17.61	7.620×10^{-2}	5.17	3.942×10^{-1}	4.87
	p-xylene	8	10.79	2.858×10^{-2}	7.62	2.881×10^{-1}	6.92
n-decane	argon	3	12.26	-5.149×10^{-2}	5.01	-4.105×10^{-1}	5.74
	carbon tetrachloride	3	6.08	-2.744×10^{-2}	0.74	-1.265×10^{-1}	1.05

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	12-crown-4	4	13.13	-7.401×10^{-2}	2.93	-2.619×10^{-1}	2.92
	15-crown-5	4	13.95	-7.414×10^{-2}	5.15	-2.492×10^{-1}	5.19
	18-crown-6	4	11.72	-6.570×10^{-2}	2.97	-2.570×10^{-1}	2.87
	dicyclohexano-18-crown-6	4	12.10	-6.592×10^{-2}	3.01	-2.131×10^{-1}	2.23
	dicyclohexano-24-crown-8	4	16.69	-9.014×10^{-2}	3.31	-2.728×10^{-1}	2.24
	krypton	3	6.35	-1.799×10^{-2}	4.96	-9.196×10^{-2}	5.28
	tetrabutyltin	4	20.73	-1.045×10^{-1}	1.40	-4.074×10^{-1}	0.46
	tetraethyltin	4	15.00	7.229×10^{-2}	1.84	3.277×10^{-1}	0.76
	tetramethyltin	4	11.01	-5.890×10^{-2}	1.31	-2.634×10^{-1}	2.28
	tetrapropyltin	4	12.14	-5.827×10^{-2}	0.24	-2.450×10^{-1}	0.91
	s-trioxane	4	14.36	-7.347×10^{-2}	1.36	-2.888×10^{-1}	2.13
	xenon	8	8.11	5.266×10^{-3}	7.93	2.993×10^{-2}	7.87

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
2,3-dimethylbutane	benzene	11	8.77	-3.834×10^{-2}	1.65	-2.898×10^{-1}	1.64
	naphthalene	9	3.03	1.325×10^{-2}	2.07	7.908×10^{-2}	2.08
	phenanthrene	11	8.47	4.517×10^{-2}	2.90	2.503×10^{-1}	2.89
	toluene	10	5.36	-2.908×10^{-2}	1.41	-2.050×10^{-1}	1.39
n-dodecane	acetone	5	31.64	-1.441×10^{-1}	1.02	-6.070×10^{-1}	1.30
	benzene	4	26.19	-1.229×10^{-1}	0.49	-5.098×10^{-1}	0.98
	carbon dioxide	9	14.60	-7.529×10^{-2}	8.37	-3.982×10^{-1}	10.12
	carbon monoxide	9	41.76	-1.880×10^{-1}	9.32	-2.011	12.22
	n-decane	5	6.95	-3.194×10^{-2}	2.17	-1.810×10^{-1}	3.03
	n-hexadecane	5	16.88	8.487×10^{-2}	4.43	2.477×10^{-1}	2.51
	linoleic acid methyl ester	4	29.39	-1.384×10^{-1}	2.25	-3.981×10^{-1}	1.54
	naphthalene	5	3.52	-1.576×10^{-2}	1.86	-5.033×10^{-2}	1.94

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	n-octane	9	6.01	-2.991×10^{-2}	1.47	-1.354×10^{-1}	2.24
	n-tetradecane	5	6.52	-4.062×10^{-2}	3.70	-1.984×10^{-1}	3.68
	toluene	4	18.17	-9.156×10^{-2}	1.16	-3.589×10^{-1}	1.18
	1,3,5-trimethylbenzene	4	16.51	-8.181×10^{-2}	1.54	-2.505×10^{-1}	1.95
	vitamin K$_3$	4	7.82	3.672×10^{-2}	0.72	1.169×10^{-1}	0.52
	m-xylene	4	9.64	-5.135×10^{-2}	1.14	-1.651×10^{-1}	1.40
n-eicosane	carbon dioxide	5	47.89	-2.382×10^{-1}	4.71	-1.440	8.12
	carbon monoxide	5	86.18	-3.683×10^{-1}	2.88	-4.302	7.09
	n-dodecane	5	39.67	-1.805×10^{-1}	2.29	-7.710×10^{-1}	3.13
	n-hexadecane	5	14.13	-6.736×10^{-2}	2.22	-2.233×10^{-1}	3.17
	n-octane	5	48.75	-2.287×10^{-1}	3.11	-1.150	4.53
ethane	1-octene	6	14.98	6.900×10^{-2}	5.98	3.770×10^{-1}	5.69

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	1-tetradecene	9	25.34	1.333×10^{-1}	2.03	6.643×10^{-1}	1.84
n-heptane	benzene	11	12.29	-5.496×10^{-2}	2.36	-2.729×10^{-1}	2.33
	n-decane	6	0.98	8.972×10^{-4}	0.92	1.500×10^{-2}	0.88
	n-dodecane	6	7.02	3.308×10^{-2}	1.24	1.403×10^{-1}	1.51
	ethylbenzene	4	10.93	-5.637×10^{-2}	0.82	-2.098×10^{-1}	1.08
	n-hexadecane	9	20.64	1.060×10^{-1}	1.90	3.324×10^{-1}	1.46
	n-hexane	11	2.21	-9.846×10^{-3}	1.40	-4.358×10^{-2}	1.35
	n-octane	13	1.69	2.548×10^{-3}	1.66	1.155×10^{-2}	1.68
	n-tetradecane	6	2.99	1.747×10^{-2}	1.43	7.389×10^{-2}	1.49
	toluene	4	5.67	-3.162×10^{-2}	2.31	-1.548×10^{-1}	2.46
	1,3,5-trimethylbenzene	4	7.63	-3.857×10^{-2}	0.68	-1.520×10^{-1}	0.86
	2,2,4-trimethylpentane	4	9.08	-4.467×10^{-2}	0.43	-2.006×10^{-1}	0.37

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	o-xylene	4	3.32	-1.241×10^{-2}	3.24	-5.336×10^{-2}	3.30
	p-xylene	4	4.34	1.819×10^{-2}	2.10	1.268×10^{-1}	2.00
n-hexadecane	carbon dioxide	10	35.61	-1.617×10^{-1}	4.13	-5.341×10^{-1}	8.15
	carbon monoxide	10	95.40	-4.059×10^{-1}	3.31	-2.513	8.90
	n-decane	5	26.23	-1.120×10^{-1}	11.12	-4.237×10^{-1}	7.38
	n-dodecane	5	8.59	-3.198×10^{-2}	4.88	-8.363×10^{-2}	3.88
	n-octane	10	25.50	-9.798×10^{-2}	8.82	-3.417×10^{-1}	5.53
	n-tetradecane	5	13.47	-6.707×10^{-2}	7.32	-1.770×10^{-1}	5.74
n-hexane	acetone	5	14.47	-5.912E-02	2.11	-2.870E-01	2.14
	acetonitrile	7	5.84	-6.807×10^{-4}	5.81	-2.451×10^{-3}	5.81
	benzene	48	6.60	-1.905×10^{-2}	4.83	-8.948×10^{-2}	5.06
	carbon disulfide	10	10.43	4.360×10^{-2}	4.75	1.925×10^{-1}	4.75

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	carbon tetrabromide	8	8.51	-4.386×10^{-2}	5.89	-1.640×10^{-1}	5.89
	o-difluorobenzene	7	10.29	5.111×10^{-2}	1.78	2.144×10^{-1}	2.45
	p-difluorobenzene	7	10.52	5.444×10^{-2}	1.31	2.310×10^{-1}	1.75
	9,10-dimethylanthracene	8	21.59	1.159×10^{-1}	1.18	4.041×10^{-1}	1.18
	1,1′-dimethylferrocene	4	16.67	-8.488×10^{-2}	0.89	-3.721×10^{-1}	0.89
	ethylferrocene	4	13.63	-6.778×10^{-2}	0.68	-2.891×10^{-1}	0.68
	ferrocene	4	8.22	4.022×10^{-2}	0.51	1.514×10^{-1}	0.51
	n-heptane	11	5.26	-9.722×10^{-4}	5.24	-4.214×10^{-3}	5.24
	hexafluorobenzene	7	11.64	5.953×10^{-2}	1.98	2.294×10^{-1}	1.62
	indole	2	7.19	3.150×10^{-2}	1.05	1.178×10^{-1}	1.05
	linoleic acid	2	5.08	-3.200×10^{-2}	1.34	-1.194×10^{-1}	1.34
	naphthalene	21	9.44	4.035×10^{-2}	6.39	2.072×10^{-1}	6.05

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	octafluorotoluene	7	8.94	3.931×10^{-2}	1.89	1.707×10^{-1}	1.45
	n-octane	7	3.31	1.731×10^{-2}	0.43	7.335×10^{-2}	0.45
	pentafluorobenzene	7	12.75	6.206×10^{-2}	2.96	2.436×10^{-1}	1.67
	phenanthrene	15	13.36	7.797×10^{-2}	6.54	3.702×10^{-1}	6.16
	pyrene	8	28.10	-1.337×10^{-1}	1.85	-4.374×10^{-1}	1.85
	1,2,3,5-tetrafluorobenzene	7	16.09	8.534×10^{-2}	2.67	3.152×10^{-1}	3.39
	1,2,4,5-tetrafluorobenzene	7	12.63	7.153×10^{-2}	2.04	2.792×10^{-1}	2.43
	toluene	32	5.74	-1.229×10^{-2}	5.22	-7.400×10^{-2}	5.28
	1,2,4-trifluorobenzene	7	14.37	6.784×10^{-2}	2.24	2.836×10^{-1}	1.24
	1,3,5-trimethylbenzene	20	5.26	3.439×10^{-3}	5.23	1.398×10^{-2}	5.24
	vitamin k3	5	15.22	8.587×10^{-2}	2.07	3.093×10^{-1}	2.07
	m-xylene	5	3.16	6.522×10^{-3}	2.94	2.614×10^{-2}	2.95

Solvent	Solute	NDP	TLSM AARD	TLSM$_d$ $k_{12,d}$	TLSM$_d$ AARD	TLSM$_{en}$ $k_{12,en}$	TLSM$_{en}$ AARD
	p-xylene	17	7.72	2.289×10^{-2}	7.25	1.298×10^{-1}	7.27
n-octane	argon	4	16.39	-7.539×10^{-2}	3.47	-5.037×10^{-1}	4.38
	benzene	8	10.24	-5.520×10^{-2}	1.35	-2.138×10^{-1}	1.59
	carbon tetrachloride	4	2.01	-1.365×10^{-2}	0.76	-5.500×10^{-2}	0.62
	ethylbenzene	8	11.39	-5.576×10^{-2}	1.81	-2.136×10^{-1}	2.09
	n-heptane	7	5.31	-2.225×10^{-2}	0.96	-9.658×10^{-2}	0.79
	n-hexane	6	10.02	-4.571×10^{-2}	2.78	-1.847×10^{-1}	2.52
	krypton	4	7.89	-4.417×10^{-2}	4.28	-8.951×10^{-2}	4.80
	methane	4	60.89	-2.716×10^{-1}	1.95	-1.765	4.19
	tetrabutyltin	4	11.69	-7.100×10^{-2}	3.47	-2.701×10^{-1}	2.22
	tetraethyltin	5	5.32	-1.307×10^{-2}	4.66	-4.837×10^{-2}	4.61
	tetramethyltin	4	6.23	-3.458×10^{-2}	0.96	-1.418×10^{-1}	0.98

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	tetrapropyltin	4	4.83	-2.720×10^{-2}	2.19	-1.042×10^{-1}	1.70
	toluene	8	10.11	-5.243×10^{-2}	1.55	-2.347×10^{-1}	1.69
	1,3,5-trimethylbenzene	8	13.41	-6.727×10^{-2}	0.64	-2.541×10^{-1}	0.46
	xenon	8	9.46	-1.719×10^{-2}	9.14	-9.309×10^{-2}	9.32
	o-xylene	8	3.50	-1.985×10^{-2}	1.02	-7.577×10^{-2}	0.92
	p-xylene	8	3.41	1.421×10^{-2}	1.32	5.496×10^{-2}	1.39
propane	1-octene	8	17.32	8.520×10^{-2}	2.23	3.693×10^{-1}	1.82
	1-tetradecene	8	24.65	1.278×10^{-1}	2.61	5.187×10^{-1}	2.10
sulfur hexafluoride	benzene	9	14.30	-3.528×10^{-2}	8.41	-2.123×10^{-1}	8.41
	benzoic acid	6	12.32	-6.601×10^{-2}	4.99	-3.228×10^{-1}	5.03
	carbon tetrachloride	7	10.97	-5.444×10^{-3}	10.67	-2.915×10^{-2}	10.67
	naphthalene	5	15.96	7.966×10^{-2}	5.47	3.661×10^{-1}	5.60

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	toluene	11	14.37	-6.357×10^{-2}	11.39	-3.682×10^{-1}	11.39
	1,3,5-trimethylbenzene	10	11.16	-3.744×10^{-2}	10.37	-1.921×10^{-1}	10.37
	p-xylene	52	9.76	3.268×10^{-2}	7.57	1.501×10^{-1}	7.46
n-tetradecane	acridine	8	37.40	2.007×10^{-1}	23.61	7.673×10^{-1}	21.29
	argon	4	55.66	2.829×10^{-1}	37.15	9.802×10^{-1}	36.36
	benzothiophene	7	29.29	1.060×10^{-1}	17.85	5.133×10^{-1}	16.64
	carbon tetrachloride	4	64.04	3.546×10^{-1}	33.15	9.857×10^{-1}	31.35
	dibenzothiophene	8	28.93	1.041×10^{-1}	15.00	4.563×10^{-1}	14.19
	krypton	4	58.90	3.267×10^{-1}	38.16	9.843×10^{-1}	36.30
	methane	4	50.82	-4.648×10^{-2}	50.75	9.631×10^{-1}	49.83
	naphthalene	7	43.72	1.406×10^{-1}	26.51	6.127×10^{-1}	24.90
	tetrabutyltin	4	49.17	2.148×10^{-1}	37.78	7.907×10^{-1}	34.89

			TLSM	TLSM$_d$		TLSM$_{en}$	
Solvent	Solute	NDP	AARD	$k_{12,d}$	AARD	$k_{12,en}$	AARD
	tetraethyltin	4	55.67	2.731×10^{-1}	40.19	9.264×10^{-1}	37.19
	tetramethyltin	4	55.09	2.559×10^{-1}	39.67	9.249×10^{-1}	37.28
	tetrapropyltin	4	53.91	2.456×10^{-1}	38.74	8.652×10^{-1}	35.75
	xenon	8	71.70	3.204×10^{-1}	50.46	9.978×10^{-1}	48.89
2,2,4-trimethylpentane	benzene	4	31.91	-1.543×10^{-1}	1.65	-3.371	2.96
	1,3,5-trimethylbenzene	4	27.72	-1.771×10^{-1}	4.27	-2.744	5.40
	ethylbenzene	4	31.88	-1.540×10^{-1}	1.34	-2.638	1.44
	toluene	4	34.62	-1.338×10^{-1}	1.64	-3.002	2.39
	o-xylene	4	27.34	-1.240×10^{-1}	2.46	-2.540	3.73
	p-xylene	4	14.73	-7.543×10^{-2}	1.82	-2.330	1.91

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