SELF-DIFFUSION IN MOLECULAR FLUIDS AND NOBLE GASES: AVAILABLE DATA

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ABSTRACT

Experimental self-diffusivities of gases, vapors, and liquids obtained by means of tracer techniques and nuclear magnetic resonance are reviewed. The considered substances range from noble gases and simple diatomics (nitrogen, oxygen, carbon monoxide, etc.) to complex organic molecules, such as phenolphthalein dimethyl ether and 2-(α-methylbenzylamino)-5-nitropyridine, although polymers have not been included. Some comments on the applicability of neutron scattering to the determination of self-diffusion coefficients are also made. All the experimental results of the investigated systems are given as Supporting Information, whereas the references, temperatures, and pressures of these data and the main features of the measurement methods are compiled and classified.

1. INTRODUCTION

The intradiffusion coefficient can be defined as the translational motion of molecules of a component 1 across a chemically homogeneous mixture of 1 with other substances. The term "self-diffusion" ($\mathfrak{D}_{11}$) is a special case of intradiffusion where there is only one component in the system.[1] Availability of reliable experimental self-diffusivities allows the testing of theoretical intermolecular potentials for pure substances, since this transport property is easily calculable by computer simulation.[2] Additionally, the development of mathematical models for self-diffusion is interesting from a practical point of view, because they should be capable of predicting binary diffusivities,[3-6] which are necessary in the design of industrial processes involving mass transfer.

Unfortunately, reviews of self-diffusion coefficients are scarce in comparison to those of the other two transport properties (viscosity and thermal conductivity), and are included in more general works, dealing with binary (or even multicomponent) diffusivities. In the paper of

Johnson and Babb,[7] that focuses on liquid nonelectrolytes until 1956, only the self-diffusivities of 11 compounds were cited, whereas in the work of Marrero and Mason,[8] which covered almost all the low-density coefficients prior to 1970, this number increased to 20 (although part of the points were not experimentally obtained but calculated by intermolecular potentials and/or viscosities). The relatively recent book of Winkelmann[9] reported self-diffusivities of 36 fluids (both measured and calculated), including a considerable amount of the data found by Marrero and Mason.

In the present publication, we have attempted to make an overview, as extensive as possible, of all self-diffusion coefficients published to date for liquids, vapors, and gases of organic and inorganic substances, excluding polymers, ionic compounds and metals. More than 15 000 points of 360 substances have been classified in tables according to the measurement techniques, experimental conditions, and other interesting features. Furthermore, all these data are available as Supporting Information, even graphical information. Unlike previous works, we have read directly from the figures with the help of AutoCAD® 2007 when the numeric values were not given in the corresponding articles. The estimated uncertainty for these readings, after testing our procedure in papers where both tables and graphics were present, is around 1-2% (a figure generally lower than experimental precision). On the other hand, self-diffusivities estimated from membrane permeabilities (that change from membrane to membrane[10-12]) or calculated from binary diffusion, intermolecular potentials, or viscosities,[13-20] which were cited by Marrero-Mason and/or Winkelmann, have not been considered here.

CAS-numbers, molar masses, melting and boiling points, and critical properties of the compiled substances are also listed in the Supporting Information. They were taken mainly from the handbook of Yaws,[21] but also from the website of the Chemical Abstracts Service[22] and other specific references.[23-29]

2. EXPERIMENTAL PROCEDURES

2.1. Tracer methods. These techniques introduce a small amount of a chemical species which is similar (but not equal) to the molecules of the fluid whose self-diffusion is required, and measure their mobility. The chemical species, called tracer, usually differs from those of the medium by the substitution of one atom by some isotope, i.e., hydrogen by deuterium (D) or tritium (T), carbon 12 by carbon 13 (^{13}C) or 14 (^{14}C), oxygen 16 by oxygen 18 (^{18}O), etc. According to Barton and Speedy,[30] Marrero and Mason,[8] and Winkelmann,[9] the experimental ways to determine the diffusion of the tracer can be classified as closed tube or Loschmidt cell, gas chromatography, gel chromatography, liquid chromatography, interferometry, diffusion bridge, capillary leak, open ended capillary, point source technique, those based on the Dufour effect or on the Kirkendall effect, two-bulb device, back diffusion, diaphragm cell, and the fritted glass plug cell. We have also included three other procedures that were only utilized by their inventors and are not mentioned in those general works, i.e., the sheared boundary apparatus of Devell,[31] the modified capillary method of Pruppacher,[32] and the unsteady-state porous frit cell of Mitchel et al.[33,34]

Tables 1-3 compile all the substances investigated by tracer diffusion, together with the chemical species utilized, the experimental procedure, and the number of data points provided by each reference. When the same reference uses several tracers or methods, this has been divided according to the number or tracers/methods if possible. Self-diffusivities of gases (G), vapors (V), liquids (L), or even supercooled liquids (scL), are commonly given as a function of the temperature (T) and pressure (P), although occasionally, the researchers used the mass density (ρ) instead of the pressure. In order to avoid an excessive size of the tables, P and ρ are listed in the same column, and unless specified with the corresponding symbol, numbers have to be interpreted as pressures, because they are the most abundant. Additionally, many liquid self-diffusivities at atmospheric pressure (101.325 kPa) or at saturation pressure (Sat) only reported the temperature, not the pressure; so, to assign them a condition, we have supposed that diffusion coefficients were all determined at 101.325 kPa if the temperatures are lower than the normal boiling point (T_b). Fortunately, this distinction is unimportant, since the values of $\mathfrak{D}_{11}$ at saturation or at atmospheric pressure in liquids are almost the same below T_b.

Table 1 is devoted to data given numerically and Table 2 deals with points given in figures only. When the graphical self-diffusivities were correlated with simple equations in T and/or P, and asterisk (*) was placed close to the corresponding reference. There are some rare cases in which the data are given exclusively by means of formulas, and these were collected in Table 3. Nonetheless, these mathematical expressions are not of $\mathfrak{D}_{11}(T,P)$, but of the intradiffusion coefficients in binary mixtures as a function of the mole fraction (x) at a constant T and P, and therefore, we report only the calculated values for the pure fluid (x_1=1.0) and not the formulas themselves.

In Table 2, part of the points of Naghizadeh and Rice,[35] Annis et al.,[36] and Adamson and Irani[37] were those given numerically by Easteal and Woolf,[38] Weissmann and DuBro,[39] and Devell et al.,[31] respectively, but we have not included them in Table 1 since these authors obtained the numbers in the same way as us, i.e., by reading directly from the figures.

When papers do not inform about how many isotopes contained the tracer molecule, only the atom is indicated. In the case of water, we cited tritium and deuterium alone to point out that, although D_2O or T_2O are added to H_2O, the diffusing species are HDO and HTO, respectively.[40] For the krypton, xenon and neon of Groth and co-workers,[41,42] the term "several" has been chosen to designate the tracer, because the authors did not select a single isotope, but separated the gas in a light and a heavy fraction by the Clusius-Dickel technique and caused one fraction to diffuse into the other.

If available, the error (accuracy or precision of the measurements) is also included. Otherwise, the abbreviation n.a. (not available) is written. The very low uncertainties of 0.1% obtained by Vugts and co-workers for argon, nitrogen, carbon monoxide and methane[43-45] and by Trappeniers and Michels for krypton[46] only refer to relative values of $\mathfrak{D}_{11}(298.16\ \mathrm{K})/\mathfrak{D}_{11}(T)$ or $\rho\mathfrak{D}_{11}/(\rho\mathfrak{D}_{11})^0$, respectively, and the error of the absolute self-diffusivities increases to around 0.70%. The superscript "0" indicates that ρ tends to zero.

On the other hand, most of the procedures cited at the beginning of this section are absolute and do not require calibration. The diaphragm, fritted glass plug, and porous frit cells are relative and always need this, whereas the two-bulb setup can require calibration if the size

of all their parts is not well known, or if it contained a plug of porous material between the chambers. The back diffusion only needs calibration if the exact dimensions are unknown. Liquid self-diffusivities of water,[40,47] carbon tetrachloride,[48] benzene,[48,49] cyclohexane[50] and hexane, or binary diffusivities of carbon tetrachloride in cyclohexane[50] or of heavy water, potassium chloride, sodium chloride and urea in water[51-63] are the common standards for the three cells, while low density values of carbon dioxide,[64-66] argon,[65,67] hydrogen,[68] carbon dioxide+hydrogen,[69] and hydrogen+deuterium[70] are preferred for the two-bulb device. The back diffusion was only employed once by Harteck and Schmidt[68] for para-hydrogen in normal-hydrogen, and the apparatus was calibrated with diffusivities in this mixture obtained by the same authors in a closed tube. Moreover, it has to be said that some researchers did not indicate the source or values of the taken standards,[71,72] that the integral/differential aqueous diffusions of KCl from the several references are all in good agreement except those from the International Critical Tables,[61,62] Gordon[59] and Stokes[53,58] beyond 0.3 mol·L^{-1} (in fact, Stokes corrected them in a later work[73]) and that Becker et al.[74] did not calibrate their setup and only gave relative results: the absolute values included in the Supporting Information are those obtained years later by Stiel and Thodos,[75] who transformed the points of Becker into absolute ones by comparison with other $\mathfrak{D}_{11}$ available then.

With regards to the relation between the mobility of the tracer and that of the molecules of the fluid, the kinetic theory establishes that the diffusion of the isotopically labelled species in gases or vapors at low density is[3]

$$(n\mathfrak{D}_{12})^0 = \frac{3}{8[(1/2)(\sigma_1+\sigma_2)]^2}\sqrt{\frac{RT(M_1+M_2)}{2\pi M_1 M_2}} \times \frac{1}{\Omega\left(\frac{RT}{\sqrt{\varepsilon_1\varepsilon_2}}\right)} \tag{1}$$

where 1 refers to the medium and 2 to the tracer, n is the number density, σ is the molecular diameter, M is the molar mass, R is the gas constant and Ω is a function of the temperature and of the characteristic energies ε_1 and ε_2. Assuming that the isotope only changes the mass of the molecule, the self-diffusion can be obtained as

$$\frac{\mathfrak{D}_{11}}{\mathfrak{D}_{12}} = \sqrt{\frac{2M_2}{M_1+M_2}} \tag{2}$$

Equation 2 is generally considered valid, and almost all the points at low density in the Supporting Information include this correction.[36,43,64,65,67,76-84] It has been applied even to dense fluids.[75,85-89] We have maintained this mass correction in the Supporting Information, except for the methane of Mueller and Cahill[76] and the hydrogen isotopes of Amdur[81] and Mason,[36,82] since the former authors converted their data to CH_4 instead to CD_4 and the others transformed the mixtures D_2+T_2 and D_2+TH to H_2 instead of to D_2. In the case of liquids, the theoretical knowledge is lower,[90] and although some of the cited references deal with the matter for benzene and cyclohexane[91-96] and a nuclear magnetic resonance study suggested that eq 2 could be applicable too,[97] no definitive relation has been accepted and the authors reported the values of $\mathfrak{D}_{11}$ without correction. A notable exception is that of Mills[40] for water, who measured the

diffusion of HTO in H_2O, took the values of Longsworth[98,99] for HDO in H_2O and extrapolated both sets of data to pure H_2O. He did the same for heavy water as well.

Tracer techniques do not seem to be suitable for liquid helium at very low temperatures, where the quantic effects are so strong that small variations in the amount of He^3 added to the system modify the measured self-diffusivities greatly.[100-102]

Table 1. Self-Diffusion Coefficients of Several Substances, Determined by Tracer Methods, and Reported Numerically

substance	refs	tracer	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	calibration
methane	103	$^{13}CH_4$	two-bulb	1	293.16	1.01	G	2.74	not required
	65[a]	$^{13}CH_4$	two-bulb	5	90.16 to 353.16	1.01	V, G	0.60 to 8.64	not required
	104	CH_3T	Loschmidt	25	273.16 to 323.16	20.3 to 304.0	G	n.a.	not required
	105	CH_3T	point source	2	297.00	1.01	G	n.a.	not required
	106	CH_3T	gas chromatog	5	298.16	2.07 to 61.9	G	1.00 to 3.00	not required
	107	CH_3T	two-bulb (plug)	24	298.16 to 348.16	14.60 to 255.6	G	n.a.	carbon dioxide[64]
methane-d_4	76[a]	CH_4	two-bulb	3	298.20 to 382.50	1.01	G	0.28 to 0.43	not required
	45	CHD_3	two-bulb	13	233.17 to 421.80	1.01	G	0.10	argon at 298.15 K[65,67]
ethane	76[a]	C_2H_5D	two-bulb	3	298.20 to 382.50	1.01	G	0.59 to 0.95	not required
propane	108	$C_2{}^{14}CH_8$	Loschmidt	8	295.95 to 358.85	14.7 to 170.4	L	4.16 to 17.21	not required
n-pentane	109	T (1 or 2 atoms)	open ended	5	194.70 to 308.70	1.01	L	2.07 to 10.77	not required
	110	$C_4{}^{14}CH_{10}$	Loschmidt	2	273.10	1.01	V	n.a.	not required
n-hexane	111	^{14}C	open ended	1	298.16	1.01	L	2.00	not required
	112	^{14}C	diaphragm	2	298.16 and 308.16	1.01	L	0.10 to 0.20	CCl_4 in cyclohexane[50]
	91	^{14}C	diaphragm	1	298.16	1.01	L	0.50	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	71	$C_5{}^{14}CH_{14}$	diaphragm	1	298.16	1.01	L	0.40	0.5 mol·L^{-1} KCl
	113	^{14}C	open ended	1	303.20	1.01	L	0.17	not required
n-heptane	109	T (1 or 2 atoms)	open ended	7	194.70 to 369.00	1.01	L	1.92 to 16.14	not required
	114	D	interferometry	1	298.16	1.01	L	1.00	not required
	91	^{14}C	diaphragm	1	298.16	1.01	L	0.50	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	34	$C_6{}^{14}CH_{16}$	porous frit	3	293.16 to 303.16	1.01	L	5.00 to 10.00	0.5 mol·L^{-1} NaCl[53-55]
n-octane	115	^{14}C	diaphragm	4	298.16 and 333.16	1.01	L	n.a.	0.1 mol·L^{-1} KCl (1.87·10^{-9} m^2·s^{-1})
n-decane	34	$C_9{}^{14}CH_{22}$	porous frit	4	293.16 to 313.16	1.01	L	5.00 to 10.00	0.5 mol·L^{-1} NaCl[53-55]
n-dodecane	112	^{14}C	diaphragm	2	298.16 and 308.16	1.01	L	0.10 to 0.20	CCl_4 in cyclohexane[50]
	115	^{14}C	diaphragm	4	298.16 and 333.16	1.01	L	n.a.	0.1 mol·L^{-1} KCl (1.87·10^{-9} m^2·s^{-1})
isopentane	116	T	open ended	5	194.66 to 298.66	1.01	L	5.00	not required
3-methylpentane	117	^{14}C	diaphragm	3	298.13 to 308.14	1.01	L	0.50	cyclohexane[50]
isooctane	114	D	interferometry	1	298.16	1.01	L	1.00	not required
ethylene	76[a]	$C_2H_2D_2$	two-bulb	3	298.20 to 382.50	1.01	G	0.49 to 0.80	not required
	118	^{14}C	two-bulb	25	298.16 to 348.16	20.63 to 199.1	G	3.00	carbon dioxide[64]
	119	$^{14}C_2H_4$	gas chromatog.	4	254.00 to 760.00	8.00	V, G	5.00 to 9.41	not required
propene	119	$C^{14}C_2H_6$	gas chromatog.	1	327.00	8.00	V	4.35	not required
acetylene	76[a]	C_2D_2	two-bulb	3	298.20 to 382.50	1.01	V, G	0.41 to 0.75	not required
cyclopentane	116	T	open ended	5	194.66 to 319.36	1.01	L	5.00	not required
	120	T	diaphragm	1	298.15	1.01	L	0.50	0.5 mol·L^{-1} KCl[56]
cyclohexane	114	D	interferometry	1	298.16	1.01	L	1.00	not required
	50	^{14}C	diaphragm	1	298.16	1.01	L	1.00	CCl_4 in cyclohexane[50]

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
	121	^{14}C	diaphragm	1	298.16	1.01	L	0.30	0.5 mol·L^{-1} KCl[57]
	122,123	^{14}C	diaphragm	1	298.16	1.01	L	1.00 to 2.00	0.1 mol·L^{-1} KCl[58]
	124	^{14}C	diaphragm	19	288.20 to 328.20	1.01 to 821.00	L	1.00 to 2.00	CCl_4 and benzene at 298 K[48]
	92	$C_6H_{11}T$	diaphragm	1	298.16	1.01	L	0.14	0.5 mol·L^{-1} KCl[56]
	92	$C_6D_{11}T$	diaphragm	1	298.16	1.01	L	0.07	0.5 mol·L^{-1} KCl[56]
	125	$C_5{}^{14}CH_{12}$	diaphragm	6	281.70 to 313.18	1.01	L	1.24 to 3.12	benzene[49]
	125	$C_5{}^{14}CH_{12}$	gel chromatog.	2	298.18 and 308.18	1.01	L	0.41 and 0.62	not required
	93	$C_6D_{11}T_1$	diaphragm	5	281.70 to 308.18	1.01	L	1.12 to 2.89	benzene[49]
	93	$C_6D_{11}T$	gel chromatog.	2	298.18 and 308.18	1.01	L	0.21 and 0.58	not required
cyclooctane	120	T	diaphragm	1	298.15	1.01	L	0.50	0.5 mol·L^{-1} KCl[56]
benzene	126	C_6H_5D	diaphragm	4	288.16 to 318.16	1.01	L	0.53 to 2.33	0.1 mol·L^{-1} KCl[59]
	127	^{14}C	open ended	1	298.16	1.01	L	5.00	not required
	128	^{14}C	open ended	11	288.16 to 318.16	1.01 to 647	L	0.59 to 4.08	not required
	129	^{14}C	open ended	7	279.96 to 338.16	1.01	L	2.25 to 9.50	not required
	130	^{14}C	open ended	3	288.16 to 308.16	1.01	L	3.64 to 4.71	not required
	121,131	^{14}C	diaphragm	1	298.16	1.01	L	0.30	0.5 mol·L^{-1} KCl[57]
	114	D	interferometry	1	298.16	1.01	L	1.00	not required
	122,123	^{14}C	diaphragm	1	298.16	1.01	L	1.00 to 2.00	0.1 mol·L^{-1} KCl[58]
	48	^{14}C	diaphragm	4	288.20 to 318.20	1.01	L	0.20	0.5 mol·L^{-1} KCl[56]
	91	^{14}C	diaphragm	1	298.16	1.01	L	0.40	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	94	$C_5{}^{14}CH_6$	diaphragm	1	298.16	1.01	L	0.23	0.8 mol·L^{-1} urea[52]
	94	$C_4{}^{14}C_2H_6$	diaphragm	1	298.16	1.01	L	0.37	0.8 mol·L^{-1} urea[52]
	49	$C_5{}^{14}CH_6$	diaphragm	1	298.16	1.01	L	0.15	0.5 mol·L^{-1} KCl[57]
	132	$C_5{}^{14}CH_6$	diaphragm	1	298.16	1.01	L	0.20	0.8 mol·L^{-1} urea[52]
	91,95	$C_5{}^{14}CH_6$ +$C_4{}^{14}C_2H_6$	diaphragm	3	298.16	1.01	L	0.09 to 0.14	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	91,95	$C_3{}^{14}C_3H_6$	diaphragm	4	298.16	1.01	L	0.05 to 0.18	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	91,95	$C^{14}C_5H_6$	diaphragm	2	298.16	1.01	L	0.05	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	133,134	$C_5{}^{14}CH_6$	diaphragm	39	288.20 to 333.20	1.01 to 1544.00	L	0.50 to 4.00	CCl_4 and benzene[48]
	95	$C_5{}^{14}CH_6$	diaphragm	3	298.16	1.01	L	0.14	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	95	$C_4{}^{14}C_2H_6$	diaphragm	3	298.16	1.01	L	0.14 to 0.27	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	95	$C_5{}^{14}CH_6$ + $C^{14}C_5H_6$	diaphragm	1	298.16	1.01	L	0.18	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	95	$C^{14}C_5H_6$	diaphragm	7	298.16	1.01	L	0.05 to 0.23	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	71	$C_5{}^{14}CH_6$	diaphragm	1	298.16	1.01	L	0.30	0.5 mol·L^{-1} KCl
	135	$C_3{}^{14}C_3H_6$	diaphragm	3	298.16	1.01	L	0.18 to 0.59	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	135	$C^{14}C_5H_6$	diaphragm	3	298.16	1.01	L	0.09 to 0.18	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
	92,96	C_6H_5T	diaphragm	1	298.16	1.01	L	0.18	0.5 mol·L^{-1} KCl[56]
	92,96	C_6D_5T	diaphragm	1	298.16	1.01	L	0.32	0.5 mol·L^{-1} KCl[56]
	92	$C^{14}C_5H_6$	diaphragm	1	298.16	1.01	L	0.23	0.5 mol·L^{-1} KCl[56]
	125	$C_5{}^{14}CH_6$	gel chromatog.	5	280.70 to 308.18	1.01	L	0.65 to 2.84	not required

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
	93	C_6D_5T	gel chromatog.	5	280.70 to 308.18	1.01	L	0.45 to 3.54	not required
	136	^{14}C	open ended	4	290.20 to 308.20	1.01	L	0.23 to 0.32	not required
	113	^{14}C	open ended	4	298.20 to 318.20	1.01	L	0.25 to 0.33	not required
benzene-d_6	96	C_6D_5T	diaphragm	1	298.16	1.01	L	0.05	0.5 mol·L^{-1} KCl[56]
toluene	123	methyl-^{14}C	diaphragm	1	298.16	1.01	L	1.00 to 2.00	0.1 mol·L^{-1} KCl[58]
	71	$C_6{}^{14}CH_8$	diaphragm	1	298.16	1.01	L	0.75	0.5 mol·L^{-1} KCl
	137	^{14}C	diaphragm	10	298.16	1.00 to 3000.00	L	1.00 to 2.00	water,[40] CCl_4, and benzene[48]
methyl acetate	111	^{14}C	open ended	4	288.16 to 318.16	1.01	L	2.00	not required
ethyl acetate	111	^{14}C	open ended	5	288.16 to 328.16	1.01	L	2.00	not required
acetonitrile	138	$^{14}CH_3CN$	diaphragm	5	298.20	1.00 to 2533.00	L	2.00 to 2.50	CCl_4 and benzene[48]
	139,140	$^{14}CH_3CN$	open ended	1	298.16	1.01	L	< 0.50	not required
nitrobenzene	113	^{14}C	open ended	4	298.20 to 318.20	1.01	L	0.53 to 0.74	not required
tri-*n*-butyl phosphate	141	$C_{12}H_{27}O_4{}^{32}P$	open ended	1	298.16	1.01	L	0.44	not required
tetramethyl tin	142	^{14}C	open ended	5	283.16 to 303.16	1.01	L	1.20 to 2.79	not required
tetramethyl lead	143	^{14}C	open ended	4	288.16 to 303.16	1.01	L	1.95 to 2.87	not required
chloroform	144	$^{14}CHCl_3$	diaphragm	25	278.16 to 323.16	1.00 to 2750.00	L	2.00 to 3.00	water,[40] CCl_4, and benzene[48]
carbon tetrachloride	145	$CCl_3{}^{36}Cl$	open ended	6	298.16 to 323.16	1.01, 203	L	4.00	not required
	146,147	$^{14}CCl_4$	open ended	1	298.16	1.01	L	5.00	not required
	129	$^{14}CCl_4$	open ended	4	298.16 to 333.16	1.01	L	1.54 to 3.50	not required
	50	$^{14}CCl_4$	diaphragm	1	298.16	1.01	L	1.00	CCl_4 in cyclohexane[50]
	48	$^{14}CCl_4$	diaphragm	5	298.20 to 323.20	1.01	L	0.40	0.5 mol·L^{-1} KCl
	148	$^{14}CCl_4$	diaphragm	27	283.20 to 328.20	1.01 to 1475.00	L	2.00 to 4.00	0.5 mol·L^{-1} KCl,[56] CCl_4, and benzene[48]
	71	$^{14}CCl_4$	diaphragm	1	298.16	1.01	L	0.65	0.5 mol·L^{-1} KCl
dichlorodifluoromethane	149[b]	^{36}Cl	two-bulb	1	293.16	1.01	V	2.00	carbon dioxide + hydrogen[69]
1,2-dichloroethane	150	^{14}C	diaphragm	16	278.15 to 313.15	1.00 to 2830.00	L	0.50 to 2.00	0.5 mol·L^{-1} KCl,[56] CCl_4, and benzene[48]
bromoethane	126	C_2H_4DBr	diaphragm	3	288.16 to 303.16	1.01	L	4.79 to 20.0	0.1 mol·L^{-1} KCl[59]
ethyl iodide	151	$C_2H_5{}^{131}I$	open ended	1	292.51	1.01	L	0.63	not required
n-butyl iodide	151	$C_3H_7{}^{131}I$	open ended	1	292.51	1.01	L	0.52	not required
chlorobenzene	91	^{14}C	diaphragm	1	298.16	1.01	L	0.50	0.5 mol·L^{-1} KCl,[51] 1 mol·L^{-1} urea[52]
argon	152	^{41}Ar	Loschmidt	1	295.16	0.43	G	0.70	not required
	67[a]	^{41}Ar	two-bulb	5	90.16 to 326.66	1.01	V, G	0.55 to 3.60	not required
	65[a]	^{36}Ar	two-bulb	6	77.66 to 353.16	1.01	V, G	1.20 to 1.69	not required
	153	^{36}Ar	open ended	1	84.31	0.88	L	2.89	not required
	85[a]	^{37}Ar	two-bulb (plug)	10	322.56	68.9 to 294.9	G	n.a.	unspecified substance
	154	^{37}Ar	open ended	1	84.56	0.93	L	1.96	not required
	155	^{37}Ar	open ended	5	86.96 to 90.10	2.03	L	4.23 to 5.84	not required
	77[a]	^{36}Ar	capillary leak	23	77.50 to 294.00	0.12 to 0.75	V, G	2.00	not required
	43,44[a]	^{38}Ar	two-bulb	11	234.68 to 417.59	1.01	G	0.10	argon at 298.15 K[65,67]
krypton	41	Several	Loschmidt	1	293.16	1.01	G	4.30	not required

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
	78[a]	^{85}Kr	two-bulb	5	199.00 to 474.00	1.01	V,G	2.00	not required
	149[b]	^{85}Kr	two-bulb	1	293.16	1.01	G	n.a.	carbon dioxide + hydrogen[69]
	156	^{85}Kr	two-bulb (plug)	14	308.16	1.01 to 230.92	G	n.a.	with their own measurements[c]
	157	^{85}Kr	two-bulb	1	301.60	1.01	G	1.00	not required
	158	^{85}Kr	two-bulb	1	304.66	1.01	G	1.00	not required
	79[a,d]	^{85}Kr	two-bulb	9	232.00 to 470.00	1.01	G	5.00	not required
	159[b]	^{85}Kr	two-bulb	1	293.16	1.01	G	n.a.	hydrogen,[68] hydrogen+deuterium[70]
	160[b]	^{85}Kr	two-bulb	1	302.60	1.01	G	16.48	not required
	161	^{85}Kr	two-bulb	1	303.16	1.01	G	1.00	not required
	39[a]	^{86}Kr	two-bulb	6	195.70 to 1036.10	1.01	V, G	2.00 to 3.00	not required
	162	^{85}Kr	open ended	25	183.57 to 233.04	53.05 to 112.75	L, G	3.09 to 11.05	not required
	163	^{85}Kr	Loschmidt	2	297.00	0.41 and 0.94	G	7.65 and 1.92	not required
	164	^{85}Kr	open ended	39	218.80 to 274.15	5.53 to 93.48	G	3.09 to 21.80	not required
	165	^{85}Kr	Loschmidt	1	293.16	30.08	G	0.37	not required
	166	^{85}Kr	Loschmidt	15	293.00	8.55 to 30.75	G	0.11 to 0.50	not required
	119	^{85}Kr	gas chromatog.	1	336.00	8.00	G	3.51	not required
xenon	41	Several	Loschmidt	1	293.16	1.01	G	4.55	not required
	167[b]	^{131}Xe	two-bulb	1	300.46	1.01	G	2.00	not required
	168	^{131}Xe	Loschmidt	4	194.70 to 378.00	1.01	V, G	0.44 to 1.90	not required
	169	^{133}Xe	two-bulb	1	302.60	1.01	G	4.50	not required
	163	^{135}Xe + ^{133}Xe	Loschmidt	9	297.00	0.02 to 0.98	G	2.29 to 11.54	not required
oxygen	65[a]	O^{18}O	two-bulb	5	77.50 to 353.20	1.01	V, G	1.31 to 2.59	not required
	66	O^{18}O	two-bulb	2	273.00 and 318.00	1.01	G	0.57 to 0.86	not required
nitrogen	170	N^{15}N	two-bulb	1	293.16	1.01	G	3.80	not required
	65[a]	N^{15}N	two-bulb	5	77.66 to 353.16	1.01	V, G	1.85 to 3.25	not required
	66	N^{15}N	two-bulb	2	273.00 and 318.00	1.01	G	1.16 and 0.90	not required
	74	N^{15}N	two-bulb	6	293.16	20.00 to 90.00	G	0.20 to 0.87	not calibrated (relative values only)
	171[b]	N^{15}N	two-bulb	1	273.16	1.01	G	3.23	not required
	44	N^{15}N	two-bulb	13	233.17 to 421.80	1.01	G	0.10	argon at 298.15 K[65,67]
carbon monoxide	80[a]	^{14}CO	Loschmidt	4	194.70 to 373.00	1.01	G	1.00	not required
	172	^{14}CO	open ended	4	68.97 to 77.52	0.93	L	3.45 to 4.44	not required
	44	C^{18}O	two-bulb	11	233.17 to 421.80	1.01	G	0.10	argon at 298.15 K[65,67]
	44	^{13}CO	two-bulb	13	233.17 to 421.80	1.01	G	0.10	argon at 298.15 K[65,67]
carbon dioxide	65[a]	CO^{17}O + ^{13}CO^{17}O	two-bulb	4	194.66 to 353.16	1.01	V, G	0.60 to 1.96	not required
	86[a]	^{14}CO$_2$	Loschmidt	66	273.36 to 318.00	9.32 to 151.89	L,V,G	n.a.	not required
	173[b]	^{14}CO$_2$	Loschmidt	16	295.60 to 297.10	0.51 to 28.5	V	n.a.	not required
	66	CO^{18}O	two-bulb	2	273.00 and 318.00	1.01	V, G	2.08 and 1.55	not required
	64[a]	^{14}CO$_2$	Loschmidt	4	194.80 to 362.60	1.01	V, G	0.40 to 2.30	not required
	174[b]	^{14}CO$_2$	Loschmidt	24	272.90 to 398.20	132.0 to 1044.2	L, G	n.a.	not required

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
	74	$^{13}CO_2$	two-bulb	11	293.16	15.00 to 52.00	V	0.30 to 2.70	not calibrated (relative values only)
	87[a]	$^{14}CO_2$	two-bulb (plug)	27	273.16 to 373.16	6.14 to 207.5	V, G	0.30 to 0.50	carbon dioxide at 308.16 K[64-66]
	149[b]	$^{14}CO_2$	two-bulb	1	293.16	1.01	V	n.a.	carbon dioxide + hydrogen[69]
	175[b]	$^{14}CO_2$	point source	16	296.00 to 1680.00	1.01	V, G	n.a.	not required
	176	$^{14}CO_2$	two-bulb	12	233.16 to 513.16	1.01	V, G	1.00 to 2.00	not required
	79[a,d]	$^{14}CO_2$	two-bulb	9	248.00 to 362.00	1.01	V, G	5.00	not required
	105	$^{14}CO_2$	point source	2	297.00	1.01	V	n.a.	not required
	159[b]	$^{14}CO_2$	two-bulb	1	293.16	1.01	V	n.a.	hydrogen,[68] hydrogen+deuterium[70]
	177[b]	$^{14}CO_2$	point source	25	1103.00 to 1944.00	1.01	G	n.a.	not required
	88,178[a]	$^{14}CO_2$	two-bulb (plug)	99	298.16 to 348.16	2.95 to 248.9	V, G	n.a.	carbon dioxide[64]
	108	$^{14}CO_2$	Loschmidt	7	273.77 to 295.67	70.0 to 184.7	L	4.27 to 25.16	not required
	89[a,e]	$^{14}CO_2$	two-bulb	38	297.96 to 307.94	19.00 to 604.00 (ρ)	V, G	1.39 to 10.46	carbon dioxide[64-66]
uranium hexafluoride	179	$^{235}UF_6$	two-bulb	1	303.16	0.013	V	3.85	not required
	180	$^{235}UF_6$	two-bulb	21	273.16 to 306.46	0.006 to 0.022	V	n.a.	not required
carbon disulfide	181	$CS^{35}S$	fritted glass plug	28	293.00 to 313.00	203 to 10133	L	n.a.	water[47]
	72	$^{14}CS_2$, ^{35}S	diaphragm	29	268.20 to 313.20	1.00 to 3851.00	L	2.00 to 4.00	benzene and hexane
hydrogen	68	p-H_2	Loschmidt	1	273.16	1.01	G	0.19	not required
	68	p-H_2	back diffusion	2	85.00 and 20.40	1.01	G	4.65 and 1.35	hydrogen at 273.16 K [68]
	182	D_2	Loschmidt	1	288.16	1.01	G	5.20	not required
	183,184	D_2	Dufour	1	293.16	1.01	G	n.a.	not required
	70	D_2	diffusion bridge	4	65.10 to 296.00	1.01	G	2.00 to 3.00	not required
	185	D_2	Kirkendall	1	303.16	1.01	G	n.a.	not required
	186	D_2	two-bulb	5	115.00 to 295.00	1.01	G	1.50	not required
	81[a]	HT	Loschmidt	2	194.70 and 273.20	1.01	G	1.00 to 1.50	not required
	187	HT	Loschmidt	1	297.16	1.01	G	2.00	not required
	187	DT	Loschmidt	1	297.16	1.01	G	2.00	not required
	81[a]	T_2	Loschmidt	3	194.70 to 352.80	1.01	G	1.00 to 1.50	not required
	36,82[a,f]	T_2	two-bulb	3[g]	295.00	1.01	G	2.00	not required
	187	T_2	Loschmidt	1	297.16	1.01	G	2.00	not required
deuterium	81[a]	HT	Loschmidt	2	194.70 and 273.20	1.01	G	1.00 to 1.50	not required
	187	HT	Loschmidt	1	297.16	1.01	G	2.00	not required
	187	DT	Loschmidt	1	297.16	1.01	G	2.00	not required
	81[a]	T_2	Loschmidt	3	194.70 to 352.80	1.01	G	1.00 to 1.50	not required
	36,82[a,f]	T_2	two-bulb	3[g]	295.00	1.01	G	2.00	not required
	187	T_2	Loschmidt	1	297.16	1.01	G	2.00	not required
helium 4	70	^3He	two-bulb	6	14.40 to 296.00	1.01	G	2.00 to 4.00	not required
	188	^3He	two-bulb	12	76.50 to 888.30	1.01	G	2.00 to 3.00	not required
	189	^3He	gas chromatog.	6	303.00 to 806.00	1.01	G	1.31 to 4.79	not required
neon	42	Several	Loschmidt	1	293.16	1.01	G	0.42	not required

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
	65[a]	^{22}Ne	two-bulb	5	77.66 to 353.16	1.01	G	0.66 to 1.56	not required
	83[a]	^{22}Ne	two-bulb	8	77.40 to 1400.00	1.01	G	2.00 to 3.00	not required
water	47	D	diaphragm	5	273.26 to 318.16	1.01	L	0.26 to 3.61	0.1 mol·L^{-1} KCl[60,61]
	190	D	diaphragm	2	273.16 and 301.16	1.01	L	5.00	KCl[62]
	191[h]	D	open ended	7	273.16 to 328.16	1.01	L	0.70 to 2.12	not required
	191[h]	D	diaphragm	6	278.36 to 328.16	1.01	L	0.00 to 0.91	heavy water in water+heavy water[63]
	192[h]	H^{18}O	open-ended	8	274.27 to 328.16	1.01	L	1.34 to 7.96	not required
	126	D	diaphragm	4	288.16 to 318.16	1.01	L	1.47 to 2.40	0.1 mol·L^{-1} KCl[59]
	126	H^{18}O	diaphragm	2	298.16 and 318.16	1.01	L	n.a.	0.1 mol·L^{-1} KCl[59]
	193	D	diaphragm	4	288.16 to 318.16	1.01	L	0.50	unspecified substance
	194	T	fritted glass plug	30	273.00 to 323.00	1.01 to 10183	L	5.00 to 10.00	water at 298.16 K[47]
	195[h]	D	open ended	5	283.16 to 328.16	1.01	L	1.61 to 2.55	not required
	195[h]	T	open ended	5	278.16 to 318.16	1.01	L	1.30 to 3.45	not required
	195[h]	H^{18}O	open ended	8	274.27 to 328.16	1.01	L	2.10 to 6.73	not required
	196-198	H^{18}O	open ended	4	278.16 to 298.16	1.01	L	0.86 to 1.50	not required
	98	D	interferometry	2	274.16 and 298.16	1.01	L	0.10	not required
	99	D	interferometry	3	278.16 to 318.16	1.01	L	0.10	not required
	31	D	sheared boundary	1	298.16	1.01	L	0.89	not required
	31	T	sheared boundary	1	298.16	1.01	L	0.89	not required
	199	T	open ended	1	298.16	1.01	L	2.00	not required
	32	T	modified capillary	14	253.16 to 300.36	1.01	scL, L	0.92 to 5.56	not required
	200	T	diaphragm	1	306.99	1.01	L	2.00	cyclohexane or CCl_4 in cyclohexane[50]
	40	T	diaphragm	7	274.16 to 318.16	1.01	L	0.20	0.5 mol·L^{-1} KCl[56]
	201,202	T	diaphragm	54	277.20 to 318.20	1.01 to 2367.00	L	0.80	water[40]
	203	D	diaphragm	8	278.20 to 308.20	1.01	L	0.36 to 1.02	0.5 mol·L^{-1} KCl[51]
	204	D	liquid chromatog.	5	298.16 to 338.16	1.01	L	2.50	not required
	205	H^{18}O, D	diaphragm	1	298.16	1.01	L	0.09 to 0.44	0.5 mol·L^{-1} KCl[51]
	206	H^{18}O	diaphragm	8	278.44 to 323.15	1.01 to 2625.00	L	0.30 to 0.80	0.5 mol·L^{-1} KCl,[56] water[40]
	207	T	diaphragm	3	281.16 to 318.16	1.01	L	0.40 to 0.60	0.5 mol·L^{-1} KCl[56]
	139	T	open ended	1	298.16	1.01	L	< 0.50	not required
	208	H^{18}O	diaphragm	4	323.15 to 363.15	1.01	L	0.20	0.5 mol·L^{-1} KCl[56]
	208	T	diaphragm	5	298.15 to 363.15	1.01	L	0.60 to 8.00	0.5 mol·L^{-1} KCl[56]
heavy water	99	H	interferometry	3	278.16 to 318.16	1.01	L	0.10	not required
	40	T	diaphragm	3	278.16 to 318.16	1.01	L	0.20	0.5 mol·L^{-1} KCl[56]
	209	T	diaphragm	27	280.50 to 328.20	1.00 to 2370.00	L	1.00 to 2.00	water[40]
	207	T	diaphragm	3	281.16 to 318.16	1.01	L	0.40 to 0.60	0.5 mol·L^{-1} KCl[56]
ammonia	210	$^{15}NH_3$	two-bulb	4	233.00 to 353.00	1.01	V	1.11 to 3.70	not required
	84[a]	$^{15}NH_3$	Loschmidt	7	301.30 to 445.60	1.01	V	0.22 to 0.97	not required
hydrogen chloride	211	DCl	Loschmidt	1	294.96	1.01	V	1.24	not required

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
hydrogen bromide	211	DBr	Loschmidt	1	295.26	1.01	V	0.89	not required
methanol	193	$^{14}CH_3OH$, CH_3OD	diaphragm	3	288.16 to 308.16	1.01	L	0.50	unspecified substance
	127	$^{14}CH_3OH$	open ended	1	298.16	1.01	L	5.00	not required
	147	$^{14}CH_3OH$	open ended	1	313.16	1.01	L	2.83	not required
	212	$^{14}CH_3OH$	open ended	8	288.16 to 313.16	0.98 to 2942	L	0.54 to 2.66	not required
	129	$^{14}CH_3OH$	open ended	7	268.16 to 328.16	1.01	L	0.42 to 10.98	not required
	204	CH_3OD	liquid chromatog.	5	298.16 to 338.16	1.00, sat	L	2.50	not required
	213	CH_3OD	diaphragm	24	278.20 to 328.20	1.00 to 3858.00	L	0.80 to 2.50	CCl_4 and benzene[48]
	140	$^{14}CH_3OH$	open ended	1	298.16	1.01	L	< 0.50	not required
methanol-*d*	213	$^{14}CH_3OH$	diaphragm	1	298.30	1.01	L	4.00 to 5.00	CCl_4 and benzene[48]
ethanol	193	C_2H_5OD	diaphragm	3	288.16 to 308.16	1.01	L	0.50	unspecified substance
	126	C_2H_5OD	diaphragm	4	288.16 to 318.16	1.01	L	1.25 to 5.34	0.1 mol·L^{-1} KCl[59]
	127	$C^{14}CH_5OH$	open ended	1	298.16	1.01	L	5.00	not required
	146,147	^{14}C	open ended	1	298.16	1.01	L	5.00	not required
	129	$C^{14}CH_5OH$	open ended	7	279.96 to 338.16	1.01	L	0.78 to 2.94	not required
	111	^{14}C	open ended	2	298.16 and 318.16	1.01	L	2.00	not required
	204	C_2H_5OD	liquid chromatog.	5	298.16 to 338.16	1.01	L	2.50	not required
	213	$^{14}C_2H_5OH$	diaphragm	6	298.20	1.01 to 2652.00	L	n.a.	CCl_4 and benzene[48]
ethanol-*d*	213	$^{14}C_2H_5OH$	diaphragm	1	298.20	1.01	L	1.25	CCl_4 and benzene[48]
1-propanol	193	C_3H_7OD	diaphragm	4	288.16 to 318.16	1.01	L	0.50	unspecified substance
	204	C_3H_7OD	liquid chromatog.	5	298.16 to 338.16	1.01	L	2.50	not required
2-propanol	193	C_3H_7OD	diaphragm	4	288.16 to 318.16	1.01	L	0.50	unspecified substance
	204	C_3H_7OD	liquid chromatog.	5	298.16 to 338.16	1.01	L	2.50	not required
1-butanol	193	$C_4H_{11}OD$	diaphragm	3	298.16 to 318.16	1.01	L	0.50	unspecified substance
tert-butanol	193	$C_4H_{11}OD$	diaphragm	3	298.16 to 328.16	1.01	scL, L	0.50	unspecified substance
ethylene glycol	33	^{14}C	porous frit	4	298.16 to 323.16	1.01	L	2.00 to 3.00	0.0011 mol·L^{-1} NaCl[55]
aniline	136	^{14}C	open ended	5	293.20 to 313.20	1.01	L	1.08 to 2.45	not required
N-methylacetamide	214	^{14}C	open ended	5	308.16 to 333.16	1.01	L	< 5.00	not required
isobutyric acid	215	^{14}C	diaphragm	2	299.48 and 308.16	1.01	L	0.50	cyclohexane[50]

[a] Original data were only given with the mass correction of eq 2. In the Supporting Information, these corrections have not been applied only in the case of the results of Mueller and Cahill,[76] Amdur and Beatty,[81] and Mason et al.,[36,82] as explained in the text. [b] It is not clear if the reported data included the isotopic correction or not. [c] Durbin and Kobayashi[156] employed two devices: the dimensions of the first one were determined by filling it with mercury, but the second one was calibrated with the krypton measurements performed in the first apparatus. [d] Points of Wendt et al.[79] were later corrected by Annis et al.,[36] but these latter values were graphically given, and therefore, we have included them in Table 2. [e] The critical temperature and pressure for the commercial carbon dioxide utilized were 304.64 K and 74.2 bar, respectively. [f] Original values of Mason et al.[82] were later corrected by Annis et al.,[36] and only the corrected points have been included in the Supporting Information. [g] Three different apparatuses of the two-bulb type were employed. [h] These measurements of Wang[191,192] were revised and corrected in ref 195.

Table 2. Self-Diffusion Coefficients of Several Substances, Determined by Tracer Methods, and Reported Graphically

substance	refs	tracer	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	calibration
methane	35*	CHD_3	open ended	15	100.93 to 138.52	8.61 to 115.7	L	< 5.00	not required
	35*	CD_4	open ended	5	108.35 to 120.86	8.61	L	< 5.00	not required
	216*, [a]	$^{14}CH_4$	open ended	13	182.90 to 194.00	47.0	G	25 at T_c, (8 to 11) at other T	not required
n-hexane	113	^{14}C	open ended	1	298.20	1.01	L	n.a.	not required
cyclohexane	217	^{14}C, T	open ended	3	298.16 to 308.16	1.01	L	n.a.	not required
	113	^{14}C	open ended	1	298.16	1.01	L	n.a.	not required
benzene	218	^{14}C	open ended	1	298.16	1.01	L	2.00	not required
	217	^{14}C, T	open ended	4	298.16 to 313.16	1.01	L	n.a.	not required
toluene	217	^{14}C, T	open ended	3	298.16 to 308.16	1.01	L	n.a.	not required
	219	T	two-bulb (plug)	8	233.16 to 303.16	1.01	L	n.a.	apparently not required
nitromethane	218,220	$^{14}CH_3NO_2$	open ended	1	293.20	1.01	L	1.70	not required
carbon tetrachloride	220	^{36}Cl	open ended	1	293.16	1.01	L	2.00	not required
bromobenzene	218	^{14}C	open ended	1	298.20	1.01	L	5.75	not required
argon	35*	^{41}Ar	open ended	27	85.10 to 108.20	13.1 to 136.8	L	< 5.00	not required
	221[b]	^{36}Ar	capillary leak	34	Sat	33.64 to 924.55 (ρ)	L, V	5.00	not required
krypton	35*	^{85}Kr	open ended	19	118.40 to 147.10	8.59 and 39.6	L	< 5.00	not required
	36[c,d]	^{85}Kr	two-bulb	9	232.00 to 470.00	1.01	G	5.00	not required
	46	^{85}Kr	two-bulb (plug)	20	297.98	25.17 to 639.80 (ρ)	G	0.10	not required
xenon	35*	^{133}Xe	open ended	12	169.78 to 207.23	8.3 and 42.4	L	< 5.00	not required
carbon dioxide	36[c,d]	$^{14}CO_2$	two-bulb	9	248.00 to 362.00	1.01	V, G	5.00	not required
neon	222*	^{22}Ne	open ended	36	25.00 to 43.00	10.13 to 101.33	L	2.50 to 7.60	not required
water	37	$H^{18}O$	diaphragm	1	298.16	1.01	L	4.00	unspecified substance
	37	D	diaphragm	1	298.16	1.01	L	4.00	unspecified substance
ammonia	223*	NH_2D	open ended	8	212.56 to 305.66	Sat	L	3.00	not required
	223	$^{15}NH_3$	open ended	8	212.76 to 305.66	Sat	L	3.00	not required

[a] The critical temperature of this methane was 190.7 K, the critical pressure was not indicated. [b] The assumed critical constants for argon were 150.87 K and 534.62 kg·m^{-3}. [c] Original data were only given with the mass correction of eq 2. [d] These data are those of Wendt et al.[79] following a correction. Two of the nine points are given both numerically and graphically, but for the sake of clarity, all have been included in this table.

Table 3. Self-Diffusion Coefficients of Several Substances, Determined by Tracer Methods, and Reported in the Form of Equations

substance	reference	tracer	method	*T*/ K	*P*/ bar	$10^9 \cdot \mathfrak{D}_{11}$ / $(m^2 \cdot s^{-1})$	state	% error	calibration
benzene	113	^{14}C	open ended	288.80	1.01	1.963	L	1.12	not required
n-hexane	113	^{14}C	open ended	288.60	1.01	3.558	L	3.54	not required
				288.80	1.01	3.710	L	2.69	
				293.50	1.01	3.932	L	2.44	
				308.20	1.01	5.082	L	1.10	
cyclohexane	113	^{14}C	open ended	288.60	1.01	0.926	L	4.43	not required
				293.50	1.01	1.183	L	2.28	
				303.20	1.01	1.832	L	1.47	
n-hexane	132	$C_5{}^{14}CH_{14}$	diaphragm	298.16	1.01	4.1054 / 4.0955	L	0.20	0.8 $mol \cdot L^{-1}$ urea[52]
cyclohexane	132	$C_5{}^{14}CH_{12}$	diaphragm	298.16	1.01	1.4354 / 1.435	L	0.20	0.8 $mol \cdot L^{-1}$ urea[52]

2.2. Nuclear Magnetic Resonance. The estimation of self-diffusion coefficients by nuclear magnetic resonance began with the spin-echo method of Hahn,[224] as developed by Carr and Purcell.[225] According to these authors, in the presence of a steady-field gradient (SFG), a 90º pulse at time 0 followed by a single 180º pulse at time τ generates a "spin echo" of atomic nuclei at time 2τ. The amplitudes of the echo immediately after the 90º pulse and at the time 2τ, $A_{(0)}$ and $A_{(2\tau)}$ respectively, are related by

$$A_{(2\tau)} = A_{(0)} \exp\left[-\frac{2\tau}{t_{ss}} - \frac{2}{3}\mathfrak{D}_{11}(\gamma G)^2\tau^3\right] \quad (3)$$

where γ is the gyromagnetic ratio of the studied nucleus, t_{ss} is the spin-spin relaxation time, and G is the magnetic gradient. $\mathfrak{D}_{11}$ can be derived either from a series of echoes obtained at constant G under variation of τ or at constant τ by applying different gradient values.[226,227]

For measurements of diffusion constants below about $1 \cdot 10^{-7}$ $m^2 \cdot s^{-1}$, the pulsed field gradient (PFG), proposed by Stejskal and Tanner, is usually employed.[228,229] In this case, G is not applied throughout the experiment, but is switched off during the 90º and 180º pulses and during the echo, resulting in

$$A_{(2\tau)} = A_{(0)} exp\left[-\frac{2\tau}{t_{ss}} - \mathfrak{D}_{11}(\gamma G\delta)^2\left(\Delta - \frac{\delta}{3}\right)\right] \quad (4)$$

being δ the duration of the gradient pulse and Δ being the time between one pulse and other. When $\Delta = \delta = \tau$, the expression of Hahn and Carr-Purcell is recovered.

The main modification of eq 3 is the steady field gradient stimulated echo (SFGSE), which avoids the large loss of the spin-spin relaxation in a viscous fluid during the diffusion time Δ by storing the magnetization in the z direction during that time and allows the measurements of $\mathfrak{D}_{11}$ in supercooled liquids.[230] The pulsed field gradient has been more widely used and has generated numerous improvements, such as the PFG stimulated echo (PFGSE),[231] the Fourier transform extension of the PFG experiment (PFG-FT),[232] the addition of magic angle spinning to the PFG (PFG-MAS),[233] the PFG double stimulated echo (PFG-DSTE),[234] the alternating PFG (A-PFG),[235] the single-shot method using multiple gradient-recalled echoes (SS-MRE),[236] the spin-echo burst pulse sequence (SEBPS),[237] the diffusion-ordered spectroscopy incorporating bipolar pulse pairs (DOSY-BPP),[238] pulses from a gradient of the radiofrequency field (PRFFG),[239] and the one-shot experiment with PRFFG (OS-PRFFG).[240] For laser/ thermally polarized ^{129}Xe at low density, the single-shot PFG stimulated echo sequence (SS-PFGSE)[241] and the PFG multiple spin-echo (PFGMSE)[242] can be used, whereas for hyperpolarized gaseous ^{3}He, the combination of gradient pulses with nuclear magnetic imaging is preferred, both in a simple way (PFG-Im)[243] or in more elaborated sequences (e.g. fast low angle shot, FLASH).[244] Imaging is also applied to self-diffusion of liquids in the form of three different PFG (TDPFG-Im),[245] intravoxel incoherent motion imaging (IVIM),[246] diffusion-weighted contrast-enhanced Fourier acquired steady state technique (DW-CE-FAST),[247]

longitudinal eddy-current delay PFG or longitudinal encode-decode PFG (LED-PFG),[248] quick echo split imaging technique (QUEST),[249] mixed imaging sequence using spin and stimulated echoes (MISSTEC-2 or MISSTEC-4 according to the number of stimulated echoes)[250] and steady-state free precession (SSFP) pulse sequence,[251] although all these latter procedures are mainly focused to medical diagnoses.

Methods of nuclear magnetic resonance that did not use spin echoes have rarely been employed: Jonas and coworkers[252,253] determined the diffusion coefficients in two highly viscous liquids by the procedure of Burnett and Harmon, which is based on the spin-locking field dependence of the rotating-frame proton spin-lattice relaxation time,[254] and Barbe et al.[255] used the longitudinal relaxation time of ^{3}He gas oriented by optical pumping in a nonhomogeneous radiofrequency field.

Tables 4-6 compile all the investigated substances by nuclear magnetic resonance. P and ρ are displayed in one column following the same criteria as Tables 1 and 2, and the asterisks also mean that simple correlations in T and/or P are available for the graphical data. Some authors distinguish reproducibility from reliability, and then, we have placed the last parameter in italics in brackets. Numerically published alkanes of Bachl,[256] methane of Oosting and Trappeniers,[257] 2-ethylhexylbenzoate of Walker et al.,[253] and ketones and acetates of Petrowsky et al.[258] are published in figures elsewhere,[259-265] so we have only taken into account the numbers and have not added the graphical references to Table 5 nor to the Supporting Information.

If a reference reports diffusivities of the same molecule obtained by different techniques and/or resonant nuclei, we have divided the reference as well. The works of Saitoh et al.[266] and of Asahi and Nakamura[267] were also divided, but for the sake of clarity and not because of procedures or atoms: these researchers measured $\mathfrak{D}_{11}$ at constant ρ (in the probe of the nuclear magnetic resonance apparatus) and temperatures above and below the critical one (T_c). However, for the subcritical temperatures, most of the conditions correspond to the L-V coexistence zone, the densities are not those initially fixed, and the observed diffusion coefficient is an average value over the liquid and vapor, since the spin echoes from both phases were taken into account (so, we utilized the term "biphasic" to define the state). Notwithstanding this, a part of these coefficients are very close to those of the saturated liquid, due to the fact that the echo of the vapor decays much faster than the liquid except in the vicinity of T_c.

When there is a peculiarity in the experimental procedure, this has been indicated between parentheses: SS-PFGSE(pol) and FLASH(hyp) point out that the methods have been applied to polarized or hyperpolarized atoms, as previously said; the terms SFG(constant G) and SFG(constant τ) mean that the authors distinguish between points measured at constant G under variation of τ from those determined at constant τ by applying different gradient values; SFG(set 1) and SFG(set 2) take into account the divison of the data in two sets due to accuracy or equipment differences; H(-CH_3) and H(ring) refer to the protons of the methyl group of toluene and to the protons of the aromatic ring, respectively; SFG(2.5 mm), SFG(3 mm), SFG(8 mm), SFG(10 mm), SFG(6 $cm^2 \cdot g^{-1}$) and SFG(80 $cm^2 \cdot g^{-1}$) are the internal diameters or specific densities of the probes where Gaines et al.[268] and Hausser et al.[269] placed the samples of helium

3 and water/benzene, respectively, in order to know if the size of these cells restricted the molecular mobility; finally, PFG(Δ=40,*G*=239) and other similar expressions show the time between one pulse and another (in ms) and the magnetic gradient (in gauss/cm) because the authors changed these during the experiments to investigate the influence of both parameters in the self-diffusion of the same compound.

Occasionally, a paramagnetic substance is purposely added to the high-purity chemical in order to shorten the duration of the experiments (by reducing the spin-lattice relaxation time): the xenon of Ehrlich and Carr[270] and of Peereboom et al.[271] contained 0.5% and 0.5‰ of oxygen, respectively; there was 1.0% O_2 in the ethane of Noble[272,273] and 1.0 $g \cdot L^{-1}$ $Cu(NO_3)_2$ in the water of Becker et al.[249] Oxygen was also present in the cyclohexane and deuterated aniline of Anderson and Gerritz,[274] whereas the water of Lowe,[235,275] Merbolt[247] and Doran[237] was doped with $CuSO_4$, but none of these latter groups measured or indicated the amount of the corresponding impurity.

Some references included in Table 5 provide figures of $\mathfrak{D}_{11}$ vs *T* from low temperatures to supercritical conditions, but do not specify the density at which those supercritical self-diffusivities were obtained. We suspect that it could be the critical one (ρ_c), but since we cannot prove this, we have written "Sat and beyond" in the column of the pressure/density.

Table 6 exhibits the self-diffusion coefficients that are only available as mathematical expressions. All of them correspond to liquids and were determined by the SFG, except the carbon tetrachloride of Fischer and Weiss,[23] that could be measured by PFG as well. We have placed here ten of the twenty-one substances analyzed by Samigullin,[276] which were also represented graphically, but are not readable due to some deformation in the y-axis of the figures (and detected because a considerable disagreement between the obtained values and those calculated by the formulas). Unlike Table 3, where there were no functions of *T* and/or *P*, all data in this table are given in terms of activation energies ($E_{\mathfrak{D}}$), activation volumes ($V_{\mathfrak{D}}$) and preexponential factors ($\mathbb{D}$), defined as

$$E_{\mathfrak{D}} = -R\left[\frac{\partial \ln \mathfrak{D}_{11}}{\partial (1/T)}\right]_P \tag{5}$$

$$V_{\mathfrak{D}} = -RT\left[\frac{\partial \ln \mathfrak{D}_{11}}{\partial P}\right]_T \tag{6}$$

$$\mathbb{D} = \lim_{\substack{T\to\infty \\ P\to 0}} \mathfrak{D}_{11} \tag{7}$$

$\mathbb{D}$ is commonly replaced by a value of $\mathfrak{D}_{11}$ at atmospheric pressure and at one reference temperature. If $E_{\mathfrak{D}}$ or $V_{\mathfrak{D}}$ are not constant, we have indicated the temperatures or pressures at which they were determined, so simple interpolations can be done to solve the formulas. In the case of 1,3,5-trimethyl benzene and tetramethyl tin, the activation parameters are complex polynomials in both *T* and *P*, and therefore, in order to spare the reader the integration process, we have put the corresponding $\mathfrak{D}_{11}(T,P)$ as footnotes.

With regards to the paper of Hertz and Radle,[277] who were the first to see the characteristic pressure dependence of water at low temperatures, we have not included this anywhere because results were described in a qualitative way, i.e., they only claimed that the experimental error was around 10%, that $\mathfrak{D}_{11}$ decreased monotonously with pressure at 298.16 K, and that it went through a maximum at 273.16 K ($\mathfrak{D}_{11}$ increased from atmospheric pressure to a value (10 to 20) % higher at 147.1 MPa and then decreased to the unspecified atmospheric self-diffusion at 294.2 MPa). Later, other researchers also established the maximum at 298.16 K.

The last column of each table reports the way in which the magnetic gradient is evaluated. The accuracy in the values of $\mathfrak{D}_{11}$ is dependent on the accuracy in the knowledge of *G*, that is usually estimated in four ways:[278-282] (i) theoretically, from the known dimensions, geometry, number of turns of wire in the coil and current applied; (ii) by measuring the changes in the magnetic field when a small sample (commonly, water) is placed at different locations; (iii) by calibration (Cal) with a substance of known self-diffusion; and (iv) by the shape of the spin echo after the 90º pulse, which for cylindrical probes is related to the first-order Bessel function. Dawson et al.[283] and Khoury et al.[284] cited the use of a "flux-gate magnetometer" for this task by a procedure which is very close to the second way; that is, the apparatus indicates the values of the magnetic field along the axis of coils, and *G* is calculated with these data. For the methods of Burnett and Harmon[254] and Barbe et al.,[255] the determination of *G* is not required.

The most employed standard for calibrating *G* is the water of Mills,[40] whose self-diffusivities at (274.16 to 318.16) K and atmospheric/saturation pressure were considered the most reliable and precise ones by Weingärtner in his classical paper of 1982.[285] For higher temperatures and pressures, Weingärtner recommended the data of Krynicky et al.[286] in the ranges (343.2 to 498.2) K, (sat to 170) MPa and of Harris and Woolf[287] at (277.15 to 333.15) K and (0.1 to 301.8) MPa. The tracer diffusivities of benzene of Collings and Mills,[48] available from (288.20 to 318.20) K, are also quite used, but they are preferred for "control", a step which sometimes follows the calibration and consists in measuring the self-diffusion coefficients of other substances whose values are also known in order to ensure the goodness of the calibration step.[259,288-297] Occasionally, the control is carried out with benzene at other temperatures and/or pressures,[298-304] cyclooctane[305,306] and water at different conditions to those of the calibration.[304,307] As in Tables 1 and 2, several authors did not indicate the source or values of the taken standards[29,308-314] or the way in which *G* was determined. In the case of Tofts et al.,[315] although the calibration substance is not specified, it is added that the control stage gave values of $\mathfrak{D}_{11}$ for water very close to those of Mills.

When the researchers that obtained *G* through the shape of the spin echo also reported the H_2O self-diffusion (determined in similar form) around 298.16 K, we have added a ratio of that value of water to the self-diffusion of Mills at the same temperature in brackets. If this ratio is far from the unity and is not within the experimental uncertainty, then systematic errors are possible. This is not a general rule, as can be seen for Fischer and Weiss,[23] whose self-diffusivities for water are very low, but their benzene is in perfect agreement with that of Collings and Mills.[48] The ratio of the water self-diffusivities has been also given when the magnetic gradient was evaluated by the position of a sample.

On the other hand, several question marks can be seen in the three tables. They were placed beside information that was not explicitly given in the references, but reasonably supposed by us. This is the case of Emel'yanov et al.,[316] who did not mention the experimental technique, but we attributed the SFG to these authors on the basis that two of them used it in a similar paper published some months later;[317] or of the temperature of Valiev et al.,[318] which was selected because the self-diffusion of water was identical to that measured by them at 293.16 K in another work also of the same year.[319] The temperature at which Van Gelderen et al.[236] performed their experiments was determined after comparison of their points with those of other researchers, and the pressure limit for the alkanes of McCall et al.[320] in Table 6 was established in 55.157 MPa due to the fact that this value, indicated specifically for 2,2-dimethylbutane, was the only value reported throughout the study. In the works of Chien et al.[321] and of Zur et al.[251] we were unable to estimate the temperature at which the experiments were carried out and only the term "room" has been included in the corresponding place in the table.

Additionally, O'Reilly et al.[322] did not mention the value that they obtained for water by the shape of the echo spin in his paper of 1968, but we suppose that it was $2.23 \cdot 10^{-9}$ $m^2 \cdot s^{-1}$ at 298.16 K, since they cited it in subsequent works,[323-325] and is within the 5% of the H_2O of Simpson and Carr, as the authors said. Oosting and Trappeniers did not mention it either,[257] but the gradient evaluation is so close to that described by them in a previous study,[326] where the self-diffusion of water at 298.16 K was $2.51 \cdot 10^{-9}$ $m^2 \cdot s^{-1}$ that we are almost sure that both cases are the same. With regards to the papers of McCall and co-workers, we have assigned the value of $2.33 \cdot 10^{-9}$ $m^2 \cdot s^{-1}$ at 298.66 K[327] to the two studies on paraffins,[320,328] since all the measurements were done with the same equipment within the same year (1958 – 1959). Nonetheless, this is unsuitable for later works, because they affirmed that gradient coils were altered from time to time[329] and reported a value of $2.45 \cdot 10^{-9}$ $m^2 \cdot s^{-1}$ at 298.16 K in 1967.[330] Moreover, it is not clear if the quotation of the diffusivity of Simpson and Carr at room temperature ($2.13 \cdot 10^{-9}$ $m^2 \cdot s^{-1}$) in 1959[331] and 1960[332] indicates calibration (except, obviously, for the measurements of water in Table 6) or if they simply selected it thinking that was a more accurate value within their experimental error.

Finally, several misprints and mistakes in the consulted literature have been found: Dupré et al.[333] and Anderson and Gerritz[274] said that they calibrated their devices with the water of Hausser et al.[269] at 293.16 K and with the dodecanol of McCall et al.,[334] respectively, but the points of Hausser are only available above 298.16 K and McCall did not measure $\mathfrak{D}_{11}$ for dodecanol; the helium diffusivities in the Figure 4 of Luszczynski et al.[335] are multiplied by 10^2 instead of by 10^3, glycerol points of Hrovat and Wade[280] below 313.16 K are also wrongly multiplied by 10^9 instead of by 10^8; some captions of the tables of Bachl[256] are displaced (we identified the correct disposition by comparing the numbers with the figures of the thesis); Panchenkov et al.[336] and Samigullin[276] investigated the dichloroethane, but they did not specify the isomer (1,2-dichloroethane, 1,1-dichloroethane or a mixture of both); and Fury et al.[337] calibrated their device by erroneously assuming that the pyridine of O'Reilly was pyridine-d_5 (in fact, they previously rejected a value of $1.74 \cdot 10^{-9}$ $m^2 \cdot s^{-1}$ at 303.16 K and 0.1 MPa, obtained by evaluating G through the shape of the spin echo, which is in good agreement with the

diffusivities of Holz et al.[97] for the deuterated compound), so their results for pyridine-d_5 are higher than expected.

Table 4. Self-Diffusion Coefficients of Several Substances, Determined by Nuclear Magnetic Resonance, and Reported Numerically

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
methane	338	H	SFG	10	91.00 to 109.00	1.01	L	8.10	Cal.(water at 298.16 K[339])
	340	H	SFG	19	298.16 to 364.27	67.71 to 173.4	G	1.00	shape
	283	H	SFG	83	154.50 to 353.80	9.72 to 415.4	L,V,G	6.00	flux-gate magnetometer
	257	H	SFG	130	90.92 to 307.69	9.464 to 452.4 (ρ)	L,V,G	2.00[341]	shape (1.0918?[326])
	342	H	SFG	65	223.16 to 323.16	31.50 to 1730.00	G	2.00	Cal.(water[40] and benzene[48] at several T)
	343	H	SFG	36	110.00 to 298.15	20.76 to 2215.80	L, G	2.00	shape (1.0400)
	288	H	PFG-FT	45	295.0 to 454.00	110.00 to 2070.00	G	1.00 to 2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	308	H	PFG	6	303.30, 333.10	300.00 to 500.00	G	5.00	Cal.(water)
methane-d_4	344	D	PFG	70	143.00 to 454.00	210.00 to 2070.00	L, G	5.00	Cal.(heavy water at 298.16 K[345])
ethane	288	H	PFG-FT	65	136.00 to 454.00	250.00 to 2000.00	L, G	1.00 to 2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	308	H	PFG	6	303.30 and 333.10	300.00 to 500.00	L, G	5.00	Cal.(water)
propane	288	H	PFG-FT	95	112.00 to 453.00	Sat to 2000.00	L, G	1.00 to 2.00 *(5.0)*	Cal.(water at 298.16 K[40])
propane-d_8	340	D	SFG	16	298.16 to 358.72	42.68 to 173.4	L	5.00	shape
n-butane	256	H	SFG	49	150.00 to 541.00	Sat to 2000.00	L, G	3.00 (*10.0*)	Cal.(water[285])
n-pentane	346	H	n.a.	51	293.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
	256	H	SFG	44	145.00 to 450.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
	347	H	PFG-FT	1	298.16	1.01	L	n.a.	n.a.
n-hexane	336	H	SFG	1	298.16	1.01	L	2.43	shape (1.0309)
	348	H	SFG	1	295.16	1.01	L	5.00	n.a.
	349	H	SFG	59	223.15 to 333.15	1.00 to 3938.00	L	1.50 *(2.5)*	shape (0.9900 to 1.0100)
	256	H	SFG	42	188.00 to 455.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
	347	H	PFG-FT	2	298.16, 323.16	1.01	L	n.a.	n.a.
	345	H	PFG	1	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at 298.16 K)
	308	H	PFG	6	303.20 and 333.00	300.00 to 500.00	L	5.00	Cal.(water)
	350	H	SFG	10	288.16 to 318.16	Sat to 600.00	L	3.00	Cal.(water + heavy water[207])
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	309	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	310	H	PFG	5	303.16 to 323.16	1.01	L	8.00	Cal.(water at several T)
n-heptane	311	H	PFG	1	300.00	1.01	L	n.a.	Cal.(water), theory
	336	H	SFG	1	298.16	1.01	L	2.50	shape (1.0309)
	346	H	n.a.	55	293.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
	349	H	SFG	3	195.50 to 299.70	1.01	L	1.50 *(2.5)*	shape (0.9900 to 1.0100)
	256	H	SFG	8	187.00 to 365.00	Sat	L	3.00 (*10.0*)	Cal.(water[285])
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
n-octane	336	H	SFG	1	298.16	1.01	L	1.45	shape (1.0309)
	348	H	SFG	1	295.16	1.01	L	5.00	n.a.

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	256	H	SFG	5	223.00 to 395.00	Sat	L	3.00 (*10.0*)	Cal.(water[285])
	137	H	SFG	43	248.11 to 348.16	1.00 to 3608.00	L	1.00 *(2.0)*	Cal.(water[40] and benzene[48] at several *T*)
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	308	H	PFG	6	303.30 and 333.00	300.00 to 500.00	L	5.00	Cal.(water)
	350	H	SFG	10	288.16 to 318.16	Sat to 600.00	L	3.00	Cal.(water + heavy water[207])
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-nonane	346	H	n.a.	55	293.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
	256	H	SFG	6	226.00 to 406.00	Sat	L	3.00 (*10.0*)	Cal.(water[285])
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-decane	256	H	SFG	36	248.00 to 448.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	352	H	PFG[312]	1	298.00	1.01	L	10.00	Cal.(hexane and hexadecane[312])
	308	H	PFG	6	303.30 and 333.00	300.00 to 500.00	L	5.00	Cal.(water)
	350	H	SFG	10	288.16 to 318.16	Sat to 600.00	L	3.00	Cal.(water + heavy water[207])
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-undecane	346	H	n.a.	55	293.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-dodecane	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	350	H	SFG	10	288.16 to 318.16	Sat to 600.00	L	3.00	Cal.(water + heavy water[207])
	307	H	PFG	6	278.16 to 328.16	1.01	L	1.00	Cal.(water at 298.16 K[40,345])
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-tridecane	346	H	n.a.	50	293.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-tetradecane	318	H	SFG	1	293.16 ?	1.01	L	n.a.	shape (1.0578)
	348	H	SFG	1	295.16	1.01	L	5.00	n.a.
	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	345	H	PFG	1	298.16	1.01	L	1.78	Cal.(water[40] and benzene[48] at 298.16 K)
	307	H	PFG	5	288.16 to 328.16	1.01	L	1.00	Cal.(water at 298.16 K[40,345])
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-pentadecane	346	H	n.a.	52	293.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-hexadecane	289	H	PFG-FT	62	313.50 to 472.50	1.00 to 6000.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	353	H	SFG	25	298.16 to 348.16	1.00 to 2792.00	L	2.50	Cal.(water[40] and benzene[48] at several *T*)
	315	H	PFG	3	293.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
n-heptadecane	346	H	n.a.	44	303.00 to 353.00	1.00 to 2450.00	L	4.00 to 5.00	n.a.
n-heneicosane	354	H	PFG	9	310.16 to 333.16	1.01	scL, L	5.00	n.a.

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
n-tricosane	354	H	PFG	7	316.16 to 338.16	1.01	scL, L	5.00	n.a.
n-tetracosane	352	H	PFG[312]	3	333.00 to 405.00	1.01	L	10.00	Cal.(hexane and hexadecane[312])
	354,355	H	PFG	8	318.16 to 338.16	1.01	scL, L	5.00	n.a.
n-triacontane	289	H	PFG-FT	63	356.50 to 469.00	1.00 to 6000.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
n-dotriacontane	354	H	PFG	8	338.16 to 358.16	1.01	scL, L	5.00	n.a.
n-tetratriacontane	354	H	PFG	8	341.66 to 363.16	1.01	scL, L	5.00	n.a.
n-pentacontane	289	H	PFG-FT	46	375.00 to 473.00	1.00 to 5500.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
n-octaheptacontane	289	H	PFG-FT	35	403.00 to 473.00	1.00 to 4500.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
n-tetrapentacontahectane	289	H	PFG-FT	24	412.00 to 473.00	1.00 to 3500.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
isopentane	356	H	PFG-FT	22	298.00 to 328.00	1.00 to 2000.00	L	3.00	n.a.
2,2-dimethylbutane	256	H	SFG	38	185.00 to 450.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
2,3-dimethylbutane	309	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
	256	H	SFG	42	145.00 to 453.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
	309	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
2-methylpentane	309	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
3-methylpentane	309	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
2,2,3-trimethylbutane	256	H	SFG	30	251.00 to 450.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
3-methyl heneicosane	312	H	PFG, PFGSE	5	298.00 to 373.00	1.01	L	10.00	Cal.(hexane and hexadecane)
4-methyl docosane	312	H	PFG, PFGSE	5	298.00 to 373.00	1.01	L	10.00	Cal.(hexane and hexadecane)
9-methyl tricosane	312	H	PFG, PFGSE	5	298.00 to 373.00	1.01	L	10.00	Cal.(hexane and hexadecane)
10-*n*-hexyl nonadecane	312	H	PFG, PFGSE	7	273.00 to 373.00	1.01	L	10.00	Cal.(hexane and hexadecane)
squalane	312,352	H	PFG, PFGSE	4	293.00 to 372.00	1.01	L	10.00	Cal.(hexane and hexadecane)
ethylene	357	H	n.a.	64	123.15 to 298.15	20.44 to 2721.68	L, G	0.50 to 1.50	n.a.
cis-butene	256	H	SFG	43	150.00 to 443.00	Sat to 2000.00	L, G	3.00 (*10.0*)	Cal.(water[285])
trans-butene	256	H	SFG	40	176.00 to 441.00	Sat to 2000.00	L, G	3.00 (*10.0*)	Cal.(water[285])
2-butyne	256	H	SFG	32	241.00 to 443.00	Sat to 2000.00	L	3.00 (*10.0*)	Cal.(water[285])
cyclopropane	358	H	SFG	3	181.50 to 297.00	Sat	L	5.07 to 5.43	Cal.(water[40] at 297 K, pentane[320] at others)
cyclopentane	120	H	SFG	1	298.15	1.01	L	1.00	Cal.(water[40] and benzene[48] at several T)
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	356	H	PFG-FT	21	298.00 to 328.00	1.00 to 2000.00	L	3.00	n.a.
	345	H	PFG	1	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at 298.16 K)
	234	H	PFG-DSTE	1	298.16	1.01	L	0.65	Cal.(water + heavy water[345])
methylcyclopentane	309	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
cyclohexane	360	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874[361])
	362	H	SFG	1	323.16	1.01	L	7.00	n.a.
	330	H	SFG	1	298.16	1.01	L	< 5.00	shape (1.0657)
	363	H	SFG	2	298.16 and 333.16	1.01	L	< 5.00	shape (1.0450[364])
	365	H	SFG	13	293.20 to 523.20	Sat	L	3.00	shape (1.0309)
	366	H	SFG	1	301.16	1.01	L	8.00	shape (0.9255)

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	367	H	SFG	39	313.00 to 383.00	1.00 to 2140.00	L	n.a.	n.a.
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	245[a]	H	TDPFG-Im	1	295.16	1.01	L	15.57	Cal.(H_2O and glycerol) but relative values only
	368	H	PFG-FT	1	298.16	1.01	L	0.68	Cal.(water at 298.16 K[40])
	345	H	PFG	1	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at 298.16 K)
	369	H	PFG	1	298.16	1.01	L	n.a.	shape (0.9830)
	370	^{13}C	PRFFG	1	298.16	1.01	L	1.98	Cal.(benzene at 298.16 K, 2.21·10^{-9} m^2·s^{-1})
	307	H	PFG	5	288.16 to 328.16	1.01	L	1.00	Cal.(water at 298.16 K[40,345])
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	371	H	PFG	4	298.16 to 313.16	1.01	L	n.a.	n.a.
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	372	H	PFG	12	303.16 to 523.16	Sat	L	5.00	Cal.(water at 303.16 K[40])
	373	H	PFG	36	423.16 to 673.16	4.90 to 147.00 (ρ)	V, G	5.00	Cal.(water at 303.16 K[40])
	310	H	PFG	4	308.16 to 323.16	1.01	L	8.00	Cal.(water at several *T*)
methylcyclohexane	336	H	SFG	1	298.16	1.01	L	2.17	shape (1.0309)
	365	H	SFG	13	293.20 to 523.20	Sat	L	3.00	shape (1.0309)
	374	H	SFG	30	203.00 to 298.00	1.00 to 5000.00	L	5.00 to 15.00	Cal.(cyclohexane at 313.16 K[124])
cycloheptane	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
cyclooctane	120	H	SFG	1	298.15	1.01	L	1.00	Cal.(water[40] and benzene[48] at several *T*)
	345	H	PFG	1	298.16	1.01	L	0.90	Cal.(water[40] and benzene[48] at 298.16 K)
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
	234	H	PFG-DSTE	1	298.16	1.01	L	0.91	Cal.(water + heavy water[345])
benzene	360	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874[361])
	375	H	SFG	1	296.16	1.01	L	n.a.	n.a.
	376	H	SFG	5	288.20 to 328.20	1.01	L	< 5.00	shape
	330	H	SFG	2	298.16	1.01	L	< 5.00	shape (1.0657)
	363	H	SFG	2	298.16, 333.16	1.01	L	< 5.00	shape (1.0450[364])
	377	H	PFG	12	278.16 to 373.16	Sat	scL, L	n.a.	n.a.
	365	H	SFG	14	293.20 to 523.20	Sat	L	3.00	shape (1.0309)
	378	H	SFG	4	288.16 to 318.16	1.01	L	n.a.	shape (0.9830)
	348	H	SFG	1	295.16	1.01	L	5.00	n.a.
	366	H	SFG	1	301.46	1.01	L	8.00	shape (0.9255)
	286	H	SFG	1	298.16	1.01	L	5.00	shape (1.0000)
	379	H	PFG-FT	1	298.16	1.01	L	0.89	Cal.(water at 298.16 K[40])
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	368	H	PFG-FT	1	298.16	1.01	L	1.33	Cal.(water at 298.16 K[40])
	278	H	SFG	1	300.66	1.01	L	2.00	shape (1.0168)

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	279	H	PRFFG	1	298.16	1.01	L	n.a.	sample location + correction (1.1309)
	266	H	SFG	1	293.16	1.01	L	5.10	shape
	369	H	PFG	1	298.16	1.01	L	n.a.	shape (0.9830)
	240	H	PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	240	H	OS-PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	267	H	SFG	1	298.00	1.01	L	n.a.	shape
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	372	H	PFG	12	303.16 to 523.16	Sat	L	5.00	Cal.(water at 303.16 K[40])
	373	H	PFG	47	423.16 to 673.16	7.20 to 208.00 (ρ)	V, G	5.00	Cal.(water at 303.16 K[40])
	310	H	PFG	5	303.16 to 323.16	1.01	L	8.00	Cal.(water at several T)
benzene-d_6	380[b]	D	SFG	35	303.00 to 433.00	1.00 to 4544.00	L	n.a.	shape
	345	D	PFG	1	298.16	1.01	L	0.30	Cal.(water + heavy water[99,207])
	97	D	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
toluene	381	H	SFG	12	158.76 to 328.76	1.01	scL, L	5.00 to 10.00	n.a.
	381	H	PFGSE	5	145.56 to 189.26	1.01	scL	5.00 to 20.00	n.a.
	381	H	PFG	3	146.66 to 159.06	1.01	scL	20.00	n.a.
	365	H	SFG	14	293.20 to 523.20	Sat	L	3.00	shape (1.0309)
	382	H	n.a.	3	293.16 to 313.16	1.01	L	5.00	n.a.
	348	H	SFG	1	295.16	1.01	L	5.00	n.a.
	383	H	PFG	10	298.16 to 388.16	1.01, sat	L	1.00 to 6.00 *(10.0)*	Cal.(cyclohexane at 298.16 K, 1.47·10^{-9} m^2·s^{-1})
	137	H	SFG	43	219.55 to 323.19	1.00 to 2488.00	L	1.00 *(2.0)*	Cal.(water[40] and benzene[48] at several T)
	240	H	PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	240	H	OS-PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
toluene-d_8	384	D	SFG	14	573.16 to 723.16	100.00 to 1000.00	L, G	10.00 to 20.00	Cal.(toluene at 298.16 K[323,381])
o-xylene	348	H	SFG	1	295.16	1.01	L	5.00	n.a.
mesitylene	385	H	SFG	15	298.15 and 313.15	1.00 to 2812.00	L	2.00	Cal.(water[40] and benzene[48] at several T)
o-terphenyl	386	H	SFG	26	318.16 to 448.16	1.01	scL, L	n.a.	shape
dimethyl ether	290	H	PFG-FT	40	184.50 to 458.00	500.00 to 2000.00	L, G	1.00 to 3.00 *(5.0)*	Cal.(water at 298.16 K[40])
diethyl ether	381	H	SFG	6	167.16 to 287.36	1.01	L	5.00 to 10.00	n.a.
1,2-dimethoxy ethane	381	H	SFG	9	182.16 to 363.16	1.01	scL, L	5.00 to 10.00	n.a.
	387[c]	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
diethoxy methane	381	H	SFG	7	188.56 to 333.16	1.01	scL, L	5.00 to 10.00	n.a.
1,2-diethoxy ethane	387[c]	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
diglycole dimethyl ether	381	H	SFG	3	258.46 to 333.163	1.01	L	5.00 to 10.00	n.a.
	381	H	PFGSE	2	176.16 and 179.26	1.01	scL	20.00	n.a.
	381	H	PFG	11	181.56 to 253.16	1.01	scL, L	5.00 to 20.00	n.a.
	387[c]	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
triglyme	387[c]	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
tetrahydrofuran	361	H	SFG	1	298.16	1.01	L	8.00	shape (1.0874)
	381	H	PFG	9	174.36 to 333.16	1.01	L	5.00 to 10.00	n.a.
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
tetrahydrofuran-d_8	97	D	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
tetrahydropyran	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
1,3-dioxolane	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
dioxane	388	H	SFG	3	300.16 to 347.16	1.01	L	1.00 to 5.00	shape
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	245[a]	H	TDPFG-Im	1	295.16	1.01	L	8.90	Cal.(H_2O and glycerol) but relative values only
	245	H	PFG-FT	1	295.16	1.01	L	7.86	Cal.(cyclohexane at 295.16 K, 1.47·10^{-9} m^2·s^{-1})
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	307	H	PFG	5	288.16 to 328.16	1.01	L	1.00	Cal.(water at 298.16 K [40,345])
	234	H	PFG-DSTE	1	298.16	1.01	L	0.64	Cal.(wáter + heavy water[345])
dioxane-d_8	307	D	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
acetone	318	H	SFG	1	293.16 ?	1.01	L	n.a.	shape (1.0578)
	360,361	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874)
	330	H	SFG	3	298.16	1.01	L	<5.00	shape (1.0657)
	381	H	SFG	7	186.06 to 333.16	1.01, sat	L	5.00 to 10.00	n.a.
	324	H	SFG	1	298.00	1.01	L	n.a.	shape (0.9699)
	366	H	SFG	1	300.96	1.01	L	8.00	shape (0.9255)
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	245[a]	H	TDPFG-Im	1	295.16	1.01	L	15.60	Cal.(H_2O and glycerol) but relative values only
	245	H	PFG-FT	1	295.16	1.01	L	3.54	Cal.(cyclohexane at 295.16 K, 1.47·10^{-9} m^2·s^{-1})
	311	H	PFG	1	300.00	1.01	L	n.a.	Cal.(water), theory
	389	H	IVIM	1	298.16	1.01	L	15.00	n.a.
	246	H	IVIM	2	298.16	1.01	L	4.92 and 4.90	n.a.
	390	H	IVIM	1	298.16	1.01	L	4.02	n.a.
	279	H	PRFFG	1	298.16	1.01	L	n.a.	sample location + correction (1.1309)
	321	H	PFG-Imag	1	room	1.01	L	n.a.	n.a.
	236	H	SS-MRE	1	293.16?	1.01	L	6.45	n.a.
	236	H	PFG	1	293.16?	1.01	L	n.a.	n.a.
	249	H	PFG-Imag	1	291.66	1.01	L	0.49	n.a.
	249	H	QUEST	1	291.66	1.01	L	0.49	n.a.
	391	H	MISSTEC-2	2	296.16	1.01	L	>10.00	n.a.
	391	H	IVIM	2	296.16	1.01	L	> 2.00	n.a.

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	251	H	SSFP	1	room	1.01	L	n.a.	n.a.
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
acetone-d_6	97	D	PFG	3	288.16 to 308.16	1.01	L	1.0	Cal.(heavy water at 298.16 K[40])
2-pentanone	258	H	PFG	7	278.16 to 338.16	1.01	L	n.a.	Cal.(ethanol[129])
2-hexanone	258	H	PFG	8	278.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
2-heptanone	258	H	PFG	8	278.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
2-octanone	258	H	PFG	8	278.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
2-nonanone	258	H	PFG	8	278.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
2-decanone	258	H	PFG	8	278.16 to 353.16	1.01	scL, L	n.a.	Cal.(ethanol[129])
keto-acetylacetone	305	H	PFG-FT	35	243.00 to 423.00	1.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water at 293 K[40])
enol-acetylacetone	305	H	PFG-FT	35	243.00 to 423.00	1.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water at 293 K[40])
cyclohexanone	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
butyl acetate	258	H	PFG	8	273.16 to 343.16	1.01	L	n.a.	Cal.(ethanol[129])
pentyl acetate	258	H	PFG	9	273.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
hexyl acetate	258	H	PFG	9	273.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
octyl acetate	258	H	PFG	9	273.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
decyl acetate	258	H	PFG	9	273.16 to 353.16	1.01	L	n.a.	Cal.(ethanol[129])
ethyl propionate	387[c]	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
2-ethylhexyl	252	H	SFG	20	253.16 to 353.16	1.00 to 4500.00	L	3.00 to 10.00	shape
cyclohexanecarboxylate	252	H	Burnett-Harmon	5	253.16	2500.00 to 4500.00	L	30.00	not required
2-ethylhexyl benzoate	253	H	SFG	51	253.16 to 373.16	1.00 to 4500.00	L	3.00 to 10.00	shape
	253	H	Burnett-Harmon	11	253.16 to 293.16	1500.00 to 4500.00	L	30.00	not required
γ-butyrolactone	392	H	PFG	1	295.00	1.01	L	n.a.	shape
	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
γ-valerolactone	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
dimethyl carbonate	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
n-methyl hexyl carbonate	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-methyl octyl carbonate	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-methyl decyl carbonate	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-methyl dodecyl carbonate	258	H	PFG	8	288.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
ethylene carbonate	387	H	PFG	1	313.16	1.01	L	n.a.	shape (1.0000)
propylene carbonate	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
	393	H	PFG	4	283.00 to 298.00	1.01	L	<5.00	n.a.
butylene carbonate	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
acetic anhydride	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
pyridine	360,361	H	SFG	1	298.16	1.01	L	20.00	shape (1.0874)
	388	H	SFG	3	300.16 to 347.16	1.01	L	1.00 to 5.00	shape
	394	H	SFG	7	293.16 to 353.16	1.01	L	5.00	Cal.(water at 296.16 K, $2\cdot10^{-9}$ m^2·s^{-1})

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	395	H	PFG	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K, 2.5·10^{-9} m^2·s^{-1})
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
pyridine-d_5	337[b]	D	SFG	55	303.16 to 423.16	1.00 to 5000.00	L	n.a.	Cal.(pyridine at 303.16 K[396])
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
acetonitrile	360	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874[361])
	395	H	PFG	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K, 2.5·10^{-9} m^2·s^{-1})
	138	H	SFG	60	238.20 to 343.20	1.00 to 3036.00	L	2.00 to 2.50	Cal.(water[40] and benzene[48] at several T)
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	345	H	PFG	1	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at 298.16 K)
	397	H	LED-PFG	1	294.16	1.01	L	n.a.	shape (1.0452)
	237	H	SEBPS	1	300.16	1.01	L	3.00	n.a.
	240	H	PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	240	H	OS-PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	234	H	PFG-DSTE	1	298.16	1.01	L	0.92	Cal.(water + heavy water[345])
acetonitrile-d_3	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
n-heptanenitrile	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-octanenitrile	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-nonanenitrile	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-decanenitrile	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-dodecanenitrile	258	H	PFG	8	288.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
nitromethane	324	H	SFG	1	298.00	1.01	L	n.a.	shape (0.9699)
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	398[d]	H	PFG	10	251.10 to 314.10	1.01	L	1.08 to 5.55	Cal.(water at 298 K[40,285])
nitromethane-d_3	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
trimethyl amine	399	H	PFG-FT	49	174.00 to 423.00	100.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water[285])
triethyl amine	394	H	SFG	7	293.16 to 353.16	1.01	L	5.00	Cal.(water at 296.16 K, 2·10^{-9} m^2·s^{-1})
N,*N*-dimethylformamide	345	H	PFG	1	298.16	1.01	L	1.23	Cal.(water[40] and benzene[48] at 298.16 K)
	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	250	H	MISSTEC-2	2	296.16	1.01	L	14.10 and 14.56	n.a.
	250	H	MISSTEC-4	3	296.16	1.01	L	6.85 to 12.30	n.a.
	250	H	IVIM	1	296.16	1.01	L	7.00	n.a.
	306	H	PFG-FT	40	222.00 to 448.00	1.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water at 293 K[40])
	393	H	PFG	6	288.00 to 313.00	1.01	L	<5.00	n.a.
N,*N*-dimethylformamide-1-*d*	400	n.a.	SFG	29	240.25 to 313.15	1.00 to 2958.00	L	1.00 *(2.0)*	Cal.(water[40] and benzene[48] at several T)
N,*N*-dimethylformamide-d_7	97	D	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
dimethylacetamide	306	H	PFG-FT	49	255.00 to 468.00	1.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water at 293 K[40])

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
N-methyl-2-pyrrolidone	387	H	PFG	1	303.16	1.01	L	n.a.	shape (1.0000)
dimethylsulfoxide	360	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874[361])
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	247	H	PFG	1	293.00	1.01	L	n.a.	shape
	247	H	DW-CE-FAST	1	293.00	1.01	L	n.a.	n.a.
	345	H	PFG	1	298.16	1.01	L	1.37	Cal.(water[40] and benzene[48] at 298.16 K)
	397	H	LED-PFG	1	294.16	1.01	L	n.a.	shape (1.0452)
	237	H	SEBPS	1	300.16	1.01	L	3.00	n.a.
	240	H	PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	240	H	OS-PRFFG	1	298.16	1.01	L	n.a.	sample location (1.0000)
	97	H	PFG	3	288.16 to 298.16	1.01	scL, L	1.00	Cal.(water at 298.16 K[40])
	307	H	PFG	4	298.16 to 328.16	1.01	L	1.00	Cal.(water at 298.16 K[40,345])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	234	H	PFG-DSE	1	298.16	1.01	L	0.96	Cal.(water + heavy water[345])
	393	H	PFG	5	293.00 to 313.00	1.01	L	<5.00	n.a.
dimethylsulfoxide-d_6	97	D	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
trimethylphosphite	381	H	PFG	6	213.16 to 276.96	1.01	L	5.00 to 10.00	n.a.
tri-*n*-butyl phosphate	401	H, ^{31}P	SFG	1	293.16	1.01	L	10.00	n.a.
	313	H	DOSY-BPP	1	298.16	1.01	L	25.00	Cal.(*n*-pentanol)
tetramethyl silane	363	H	SFG	2	268.16 and 298.16	1.01	L	< 5.00	shape (1.0450[364])
	380	H	SFG	42	298.00 to 373.00	45.00 to 4500.00	L	n.a.	shape
octamethylcyclotetrasiloxane	402	H	SFG	7	323.00	1.00 to 584.00	L	1.00	Cal.(water[40] and benzene[48] at several *T*)
fluoromethane	298	n.a.	SFG	57	153.00 to 440.00	Sat to 2000.00	L, G	10.00	Cal.(water at (277 to 368) K[285])
trifluoromethane	403	H, ^{19}F	SFG	7	113.20 to 173.20	1.01	scL, L	8.00	Cal.(water at 298.16 K[339])
	299	n.a.	SFG	39	142.00 to 250.00	Sat to 2550.00	L	10.00	Cal.(water at (277 to 368) K[285])
	300	n.a.	SFG	75	142.00 to 433.00	Sat to 2000.00	L, G	5.00	Cal.(water at (277 to 368) K[285])
tetrafluoromethane	338	^{19}F	SFG	14	88.00 to 143.00	1.01	scL, L	8.1	Cal.(water at 298.16 K[339])
	284	^{19}F	SFG	54	243.16 to 348.16	24.72 to 449.87	G	3.00 to 6.00	flux-gate magnetometer
	291	^{19}F	PFG	69	140.00 to 432.00	Sat to 2000.00	L, G	1.00 to 2.00 *(3.0)*	Cal.(water at 298.16 K[40])
chloromethane	404	n.a.	SFG	50	186.00 to 440.00	Sat to 2000.00	L, G	3.00 *(10.0)*	Cal.(water[285])
dichloromethane	395	H	PFG	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K, 2.5·10^{-9} m^2·s^{-1})
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	404	n.a.	SFG	50	186.00 to 406.00	Sat to 2000.00	L	3.00 *(10.0)*	Cal.(water[285])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
chloroform	330	H	SFG	1	298.16	1.01	L	<5.00	shape (1.0657)
	322	n.a.	SFG	2	200.00, 300.00	1.01	scL, L	n.a.	Cal.(water[339]), shape (0.9699?[324])
	395	H	PFG	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K, 2.5·10^{-9} m^2·s^{-1})
	405	H	SFG	8	255.16 to 320.16	1.01	L	10.00	shape (1.0874[361])

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	404	n.a.	SFG	39	217.00 to 397.00	Sat to 1500.00	L	3.00 *(10.0)*	Cal.(water[285])
	144	H	SFG	45	278.16 to 348.16	1.00 to 3899.00	L	2.00 *(3.0)*	Cal.(water[40] and benzene[48] at several *T*)
	236	H	SS-MRE	1	293.16?	1.01	L	9.00	n.a.
	236	H	PFG	1	293.16?	1.01	L	n.a.	n.a.
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	234	H	PFG-DSTE	1	298.16	1.01	L	1.23	Cal.(water + heavy water[345])
carbon tetrachloride	370	^{13}C	PRFFG	1	298.16	1.01	L	5.97	Cal.(benzene at 298.16 K, 2.21·10^{-9} m^2·s^{-1})
chlorotrifluoromethane	406	n.a.	SFG	62	303.16 to 348.16	36.80 to 1883.80	G	1.00 to 2.00	Cal.(water[40] and benzene[48] at several *T*)
	292	^{19}F	PFG	69	133.00 to 433.00	Sat to 2000.00	L, G	1.00 to 2.00 *(3.0)*	Cal.(water at 298.16 K[40])
trichlorofluoromethane	407	^{19}F	SFG	13	379.00 and 460.00	107.00 to 1594.00	L	8.00	n.a.
bromotrifluoromethane	292	^{19}F	PFG	69	141.00 to 432.00	Sat to 2000.00	L, G	1.00 to 2.00 *(3.0)*	Cal.(water at 298.16 K[40])
bromoform	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
iodomethane	360	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874[361])
	381	H	SFG	5	213.16 to 294.16	1.01	L	5.00 to 10.00	n.a.
	395	H	PFG	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K, 2.5·10^{-9} m^2·s^{-1})
1,2-dichloroethane	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	150	n.a.	SFG	7	298.15	166.00 to 2795.00	7	2.00	Cal.(water[40] and benzene[48] at several *T*)
dichloroethane (*sic*)	336	H	SFG	1	298.16	1.01	L	2.27	shape (1.0309)
perfluorocyclobutane	408	^{19}F	SFG	59	323.00 to 473.00	50.00 to 1900.00	L, G	6.00	n.a.
fluorobenzene	345	H	PFG	1	298.16	1.01	L	0.84	Cal.(water[40] and benzene[48] at 298.16 K)
1,3,5-trifluorobenzene	381	H	SFG	5	262.36 to 357.16	1.01, sat	L	5.00 to 10.00	n.a.
hexafluorobenzene	363	^{19}F	SFG	3	268.16 to 333.16	1.01	scL, L	< 5.00	shape (1.0450[364])
	345	^{19}F	PFG	1	298.16	1.01	L	1.00	Cal.(fluorobenzene[345])
chlorobenzene	322[e]	H	SFG	2	250.00 and 300.00	1.01	L	n.a.	Cal.(water[339]), shape (0.9699?[324])
	324	H	SFG	1	298.00	1.01	L	n.a.	shape (0.9699)
benzotrifluoride	409	H	SFG	2	293.16 and 373.16	1.01	L	5.00	n.a.
dinitrofluoromethane	409	H	SFG	2	293.16 and 373.16	1.01	L	5.00	n.a.
1-fluoro-1,1-dinitroethane	409	H	SFG	2	293.16 and 373.16	1.01	L	5.00	n.a.
trinitrofluoromethane	409	^{19}F	SFG	2	293.16 and 373.16	1.01, sat	L	5.00	n.a.
trichloro (3,3,3-trifluoropropyl) silane	409	H	SFG	2	293.16 and 373.16	1.01	L	5.00	n.a.
trichloro (1-chloro-3,3,3-trifluoropropyl) silane	409	H	SFG	2	293.16 and 373.16	1.01	L	5.00	n.a.
trichloro (3,3,3-trifluoro-1-propen-1-yl) silane	409	H	SFG	2	293.16 and 373.16	1.01	L	5.00	n.a.
xenon	410	^{129}Xe	SFG	1	198.16	Sat	L	50.00	n.a.
	411	^{129}Xe	SFG	7	201.16 to 298.00	5.57 to 110.4	L, G	15.00 to 20.00	n.a.

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	271	^{131}Xe	SFG	33	203.00 to 343.00	59.04 to 2713.9 (ρ)	L,V,G	0.50 to 1.00	sample location
	271	^{129}Xe	SFG	38	248.00 to 343.00	147.58 to 2802.3 (ρ)	L,V,G	0.50 to 1.00	sample location
xenon 129	242	^{129}Xe	PFG(pol)	1	298.16	3.04	G	3.00	n.a.
	242	^{129}Xe	PFGMSE(pol)	1	298.16	3.04	G	n.a.	n.a.
	241	^{129}Xe	SS-PFGSE(pol)	1	298.16	3.04	G	n.a.	n.a.
carbon-^{13}C dioxide	412	^{13}C	PFG	58	273.16 to 348.16	10.34 to 498.48	L,V,G	0.70	Cal.(benzene[48,134])
	27	^{13}C	PFG	24	304.16 to 304.66	43.38 to 594.9 (ρ)	L,V,G	0.70	Cal.(benzene[48,134])
	413	^{13}C	PFG-FT	47	223.00 to 450.00	100.00 to 2000.00	L, G	2.00 *(5.0)*	Cal.(water[285])
uranium hexafluoride	314	^{19}F	SFG	7	340.16 to 371.16	Sat	L	n.a.	Cal.(water), theory, shape
molybdenum hexafluoride	314	^{19}F	SFG	7	293.16 to 351.16	Sat	L	n.a.	Cal.(water), theory, shape
tungsten hexafluoride	314	^{19}F	SFG	7	281.16 to 336.16	Sat	L	n.a.	Cal.(water), theory, shape
sulfur hexafluoride	414	^{19}F	SFG	21	223.00 to 315.00	Sat	L	5.00	Cal.(water at 298.16 K[339])
	415[f]	^{19}F	SFG	29	240.00 to 370.00	3.35 to 228.00 (ρ)	L,V,G	< 6.00	n.a.
	416	^{19}F	SFG	16	296.00 and 398.00	1000.0 to 1900.00 (ρ)	L, G	6.00	shape
	417[g]	^{19}F	SFG	28	323.16	73.01 to 1333.6 (ρ)	G	0.08 to 0.71	Cal.(water at 298.16 K[40])
carbon disulfide	370	^{13}C	PRFFG	1	298.16	1.01	L	0.46	Cal.(benzene at 298.16 K, 2.21·10^{-9} m^2·s^{-1})
hydrogen sulfide	333	H	SFG	8	192.80 to 294.10	Sat	L	2.86 to 11.11	Cal.(water at 293.16 K[269]), shape
hydrogen	418	H	SFG	3	55.50 to 90.30	1.01	G	10.00	shape
	419	H	PFG-FT	45	172.00 to 372.00	500.00 to 2000.00	G	2.00 *(5.0)*	Cal.(water at 293 K)
deuterium	419	D	PFG-FT	49	171.00 to 372.00	500.00 to 2000.00	G	2.00 *(5.0)*	Cal.(water at 293 K)
helium 3	255	^{3}He	Relaxation	1	300.00	0.0013	G	5.55	not required
	244	^{3}He	FLASH (hyp)	1	293.16	1.01	G	11.00	n.a.
	243	^{3}He	PFG-Imag (hyp)	1	293.16	7.09	G	18.78	n.a.
water	225	H	SFG	1	298.16	1.01	L	<12.00	shape
	339	H	SFG	21	273.16 to 373.16	1.01	L	<7.00	n.a.
	420	H	SFG	1	298.16	1.01	L	n.a.	shape (1.0569)
	318	H	SFG	1	293.16 ?	1.01	L	n.a.	shape (1.0578)
	326	H	SFG	1	298.16	1.01	L	0.40	theory, shape
	228	H	PFG	1	298.66	1.01	L	3.42	n.a.
	228	H	SFG	1	298.66	1.01	L	2.24	n.a.
	362	H	SFG	2	293.16 and 298.16	1.01	L	n.a.	n.a.
	330	H	SFG	1	298.16	1.01	L	<5.00	shape (1.0657)
	361	H	SFG	1	298.16	1.01	L	8.00	shape (1.0874)
	421	H	SFG, PFG	1	291.56	1.01	L	7.07	shape, sample location[422]
	365	H	SFG	1	298.16	1.01	L	3.00	shape (1.0309)
	324,325	H	SFG	1	298.16	1.01	L	2.60	shape (0.9699)
	423	H	SFG	14	242.50 to 298.20	1.01	scL, L	5.00	shape
	424	H	PFG-FT	2	285.16 and 298.16	1.01	L	9.93 and 4.26	Cal.(benzene at 298.16 K[425])

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	366	H	SFG	2	301.46 and 317.76	1.01	L	8.00	shape (0.9255)
	286	H	SFG	120	275.20 to 498.20	Sat to 1700.00	L	< 5.00	shape (1.0000)
	343	H	SFG	1	318.16	318.16	L	1.40	shape
	287	H	SFG	41	277.15 to 333.15	1.00 to 3032.00	L	2.00	Cal.(water[40] and benzene[48] at several *T*)
	235,275	H	A-PFG	1	297.06	1.01	L	4.37	shape
	426	H	SFG	1	298.16	1.01	L	2.00 to 10.00	shape (0.9221)
	280,427	H	PFG	1	299.66	1.01	L	2.53	shape
	428	H	SFG	34	673.16 to 973.16	149.00 to 1459.00	G	10.00	Cal.(water at 298.16 K[40])
	245	H	PFG-FT	1	295.16	1.01	L	1.00	Cal.(cyclohexane at 295.16 K, 1.47·10^{-9} m^2·s^{-1})
	368	H	PFG-FT	4	288.16 to 315.16	1.01	L	1.01 to 1.13	Cal.(water at 298.16 K[40])
	389	H	IVIM	1	298.16	1.01	L	10.00	n.a.
	246	H	IVIM	2	298.16	1.01	L	4.26 and 4.17	n.a.
	278	H	SFG	3	300.36 to 313.56	1.01	L	2.00	shape (1.0168)
	390	H	IVIM	1	298.16	1.01	L	4.52	n.a.
	293	H	PFG	110	203.50 to 273.00	1.00 to 4000.00	scL, L	1.00 to 2.00 *(3.0)*	Cal.(water at 298.16 K[40])
	279	H	PRFFG	1	298.16	1.01	L	n.a.	sample location (1.1309)
	247	H	PFG	1	293.00	1.01	L	n.a.	shape
	247	H	DW-CE-FAST	1	293.00	1.01	L	n.a.	n.a.
	321	H	PFG-Imag	1	room	1.01	L	n.a.	n.a.
	429	H	PRFFG	1	294.16	1.01	L	5.00	sample location
	397	H	LED-PFG	1	294.16	1.01	L	n.a.	shape (1.0452)
	369	H	PFG	1	298.16	1.01	L	n.a.	shape (0.9830)
	236	H	SS-MRE	1	293.16?	1.01	L	n.a.	n.a.
	236	H	PFG	1	293.16?	1.01	L	n.a.	n.a.
	249	H	PFG-Imag	1	291.66	1.01	L	0.49	n.a.
	249	H	QUEST	2	291.66, 298.16	1.01	L	1.03 and 1.69	n.a.
	237	H	SEBPS	1	300.16	1.01	L	3.00	n.a.
	250	H	MISSTEC-2	2	296.16	1.01	L	9.59 and 12.30	n.a.
	250	H	MISSTEC-4	3	296.16	1.01	L	5.15 to 7.50	n.a.
	250	H	IVIM	1	296.16	1.01	L	4.48	n.a.
	430	H	SFG	46	251.66 to 298.66	1.00 to 3505.00	scL, L	0.80	Cal.(water at (274.16 to 318.16) K[40])
	251	H	SSFP	1	room	1.01	L	n.a.	n.a.
	431	H	PFG	26	237.80 to 298.16	1.01	scL, L	1.00	Cal.(water at 298.16 K[40,285])
	307	H	PFG	9	288.16 to 329.16	1.01	L	1.00	Cal.(water at 298.16 K[40,345])
	315	H	PFG	4	288.16 to 302.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
	432[h]	H	PFG	21	303.16 to 673.16	70.69 to 995.7 (ρ)	L, G	1.00 to 5.00	Cal.(water at 303.16 K[40])
	433,434	H	PFG	24	473.16 to 673.16	4.10 to 54.50 (ρ)	V, G	5.00	Cal.(water at 303.16 K[40])
	372[h]	H	PFG	33	303.16 to 623.16	Sat	L	5.00	Cal.(water at 303.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	234	H	PFG-DSE	1	298.16	1.01	L	0.22	Cal.(water + heavy water[345])
heavy water	421	D	SFG, PFG	1	294.86	1.01	L	6.93	shape, sample location[422]
	325	D	SFG	1	298.16	1.01	L	3.26	shape (0.9699)
	435	D	SFG	66	283.16 to 473.16	1.00 to 9000.00	L	5.00 to 10.00	shape
	436	D	SFG	36	258.16 to 283.16	1.00 to 7000.00	L	n.a.	shape
	293	D	PFG	110	243.00 to 363.00	1.00 to 2000.00	scL, L	2.0 to 3.0 *(5.0)*	Cal.(water at 298.16 K[40])
	437	D	PFG	17	244.20 to 298.25	1.01	scL, L	0.06 to 4.35	Cal.(water at 298.16 K[40,285])
	438	D	PFG	65	234.00 to 295.00	2000.00 to 4000.00	scL, L	5.0	n.a.
	432[h]	D	PFG	22	303.16 to 673.16	97.10 to 1103 (ρ)	L, G	1.00 to 5.00	Cal.(water at 303.16 K[40])
	372[h]	D	PFG	33	303.16 to 623.16	Sat	L	5.00	Cal.(water at 303.16 K[40])
water-^{18}O	287	H	SFG	37	277.16 to 333.15	1.00 to 3043.00	L	2.00	Cal.(water[40] and benzene[48] at several T)
ammonia	439	H	SFG	10	199.16 to 240.16	1.01	L	5.00	shape
	440	H	PFG-FT	50	203.00 to 473.00	100.00 to 2000.00	L, G	2.00 *(5.0)*	Cal.(water[285])
ammonia-d_3	344	D	PFG	52	203.50 to 473.50	100.00 to 2000.00	L, G	5.00	Cal.(heavy water at 298 K[345])
hydrogen fluoride	441	n.a.	SFG	1	298.00	Sat	L	15.00	shape (0.9699)
	294	^{19}F	PFG-FT	54	195.50 to 418.70	Sat to 6000.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
deuterium fluoride	294	^{19}F	PFG-FT	57	192.90 to 373.90	Sat to 6000.00	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
hydrogen chloride	442	H	SFG(set 1)	1	248.16	Sat	L	n.a.	shape
	442	H	SFG(set 2)	3	295.16 to 323.16	Sat	L	n.a.	shape
methanol	443[a]	H	SFG	1	298.16	1.01	L	n.a.	not evaluated (relative values only)
	362	H	SFG	1	323.16	1.01	L	7.00	n.a.
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	213	H	SFG	9	278.20 and 298.20	1.00 to 2876.00	L	0.80 to 2.50	Cal.(water[40] and benzene[48] at several T)
	295	H	PFG-FT	73	154.00 to 453.00	1.00 to 2500.00	scL, L	1.00 to 2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	345	H	PFG	1	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at 298.16 K)
	97	H	PFG	3	288.20 to 308.20	1.01	L	1.00	Cal.(water at 298.16 K[40])
	444	H	SFG	30	288.00 to 580.00	Sat, 49.78 to 274.18 (ρ)	L,V,G	4.00	n.a.
	445	H	PFG	3	273.10 to 298.00	1.01	L	n.a.	Cal.(water at 298.16 K[40,285])
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	234	H	PFG-DSE	1	298.16	1.01	L	0.83	Cal.(water + heavy water[345])
methanol-*d*	360,361	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874)
	446	H	SFG	56	223.00 to 323.00	15.00 to 4905.00	L	7.00	n.a.
	213	H	SFG	67	214.30 to 343.40	1.00 to 3102.00	L	4.00 to 5.00	Cal.(water[40] and benzene[48] at several T)
	295	H	PFG-FT	69	151.00 to 455.00	1.00 to 2500.00	scL, L	1.00 to 2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	97	H, D	PFG	3	288.20 to 308.20	1.01	L	1.00	Cal.(water and heavy water at 298.16 K[40])
methanol-d_4	97,447	D	PFG	1	298.20	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
methanol-d_3	447	D, H	PFG	3	288.20 to 308.20	1.01	L	1.00	Cal.(water and heavy water at 298.16 K[40])
methanol-d_1	447	H	PFG	1	298.16	1.01	L	1.00	n.a.

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
methanol-d_2	447	H	PFG	1	298.16	1.01	L	1.00	n.a.
methan-d_2-ol-*d*	447	H	PFG	1	298.16	1.01	L	1.00	n.a.
methanol-^{13}C	447	H	PFG	1	298.16	1.01	L	1.00	n.a.
ethanol	443[a]	H	SFG	1	298.16	1.01	L	n.a.	not evaluated (relative values only)
	375	H	SFG	1	296.16	1.01	L	n.a.	n.a.
	381	H	SFG	7	189.16 to 295.86	1.01	L	5.00 to 10.00	n.a.
	381	H	PFG	4	158.66 to 296.46	1.01	scL, L	5.00 to 20.00	n.a.
	395	H	PFG	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K, $2.5\cdot10^{-9}$ m^2·s^{-1})
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	295	H	PFG-FT	71	173.00 to 437.00	1.00 to 2500.00	L	1.00 to 2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	345	H	PFG	1	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at 298.16 K)
	97	H	PFG	3	288.16 to 303.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
	445	H	PFG	3	273.10 to 298.00	1.01	L	n.a.	Cal.(water at 298.16 K[40,285])
	351	H	PFG	1	298.16	1.01	L	0.40	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
ethanol-*d*	361	H	SFG	1	298.16	1.01	L	8.00	shape (1.0874)
	448	n.a.	PFG	76	158.50 to 435.50	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
	97	H, D	PFG	1	298.16	1.01	L	1.00	Cal.(water and heavy water at 298.16 K[40])
ethanol-d_6	97	D	PFG	3	288.20 to 308.20	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
ethanol-d_5	97	H, D	PFG	3	288.20 to 308.20	1.01	L	1.00	Cal.(water and heavy water at 298.16 K[40])
1-propanol	443[a]	H	SFG	1	298.16	1.01	L	n.a.	not evaluated (relative values only)
	332,334	H	SFG	1	297.16	1.01	L	n.a.	Cal.(water[339])? shape?
	448	H	PFG	56	212.00 to 441.00	1.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane [345] at 298.16 K)
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
	449	H	PFG	9	268.16 to 355.16	1.01	L	n.a.	Cal.(water[307] and methanol, ethanol[129])
1-propanol-*d*	448	n.a.	PFG	55	189.00 to 431.00	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
2-propanol	448	H	PFG	58	221.00 to 478.00	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
2-propanol-*d*	448	n.a.	PFG	56	195.50 to 476.50	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
1-butanol	443[a]	H	SFG	1	298.16	1.01	L	n.a.	not evaluated (relative values only)
	332,334	H	SFG	1	297.16	1.01	L	n.a.	Cal.(water[339])? shape?
	379	H	PFG-FT	1	298.16	1.01	L	2.33	Cal.(water at 298.16 K[40])
	450	H	PFG-FT	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K[40])
	397	H	LED-PFG	1	294.16	1.01	L	n.a.	shape (1.0452)
	315	H	PFG	4	288.16 to 303.16	1.01	L	1.40 to 2.70	Cal.(unknown substance)
	449	H	PFG	9	268.16 to 353.16	1.01	L	n.a.	Cal.(water[307] and methanol, ethanol[129])
tert-butanol	311[i]	H	PFG	1	300.00	1.01	L	n.a.	Cal.(water), theory
	445	H	PFG	2	283.40 and 298.00	1.01	L	n.a.	Cal.(water at 298.16 K[40,285])
tert-butanol-*d*	361	H	SFG	1	298.16	1.01	L	9.50	shape (1.0874)

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
1-pentanol	450	H	PFG-FT	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K[40])
	451	H	PFG	85	206.60 to 468.60	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
	307	H	PFG	6	278.16 to 328.16	1.01	L	1.00	Cal.(water at 298.16 K[40,345])
1-pentanol-*d*	451	n.a.	PFG	59	207.80 to 471.40	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
2-pentanol	451	H	PFG	39	237.10 to 483.10	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
2-pentanol-*d*	451	n.a.	PFG	55	233.30 to 482.60	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
3-pentanol	451	H	PFG	45	242.20 to 474.50	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
3-pentanol-*d*	451	n.a.	PFG	54	237.60 to 476.90	50.00 to 2000.00	L	1.00 to 2.00 *(5.0)*	Cal.(water[40] and cyclooctane[345] at 298.16 K)
3-methyl-1-butanol	375	H	SFG	1	296.16	1.01	L	n.a.	n.a.
1-hexanol	450	H	PFG-FT	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K[40])
	449	H	PFG	9	268.16 to 353.16	1.01	L	n.a.	Cal.(water[307] and methanol, ethanol[129])
1-heptanol	450	H	PFG-FT	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K[40])
1-octanol	332,334	H	SFG	1	298.16	1.01	L	n.a.	Cal.(water[339])? shape?
	450	H	PFG-FT	1	298.16	1.01	L	n.a.	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)
	449	H	PFG	8	278.16 to 353.16	1.01	L	n.a.	Cal.(water[307] and methanol, ethanol[129])
2-fluoroethanol	452	^{19}F	PFG-FT	30	262.00 to 406.00	100.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water[40])
2,2-difluoroethanol	452	^{19}F	PFG-FT	31	242.00 to 408.00	100.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water[40])
2,2,2-trifluoroethanol	452	H	PFG-FT	43	242.30 to 402.70	100.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water[40])
	453	^{19}F	SFG	2	298.16	1.01	L	1.00	Cal.(water[40] and benzene[48] at several *T*)
ethylene glycol	393	H	PFG	3	298.00 to 318.00	1.01	L	<5.00	n.a.
	454	H	PFG-FT	5	298.00 to 318.00	1.01	L	<5.00	n.a.
1,2-propanediol	454	H	PFG-FT	4	304.00 to 318.00	1.01	L	<5.00	n.a.
1,3-propanediol	454	H	PFG-FT	4	304.00 to 318.00	1.01	L	<5.00	n.a.
1,3-butanediol	455	H	n.a.	9	227.16 to 297.36	1.01	L	n.a.	n.a.
1,4-butanediol	454	H	PFG-FT	4	304.00 to 318.00	1.01	L	<5.00	n.a.
hexylene glycol	455	H	n.a.	10	220.36 to 297.36	1.01	L	n.a.	n.a.
glycerol	228	H	PFG	1	299.16	1.01	L	8.00	n.a.
	456	H	PFG	11	283.16 to 373.16	1.01	scL, L	3.00	n.a.
	427	H	PFG	1	300.56	1.01	L	3.02	shape (0.9924)
	280	H	PFG	11	289.16 to 362.76	1.01	scL, L	n.a.	shape (0.9924)
monoamine ethanol	393	H	PFG	3	288.00 to 308.00	1.01	scL, L	<5.00	n.a.
N-methyl amine	399	H	PFG-FT	45	203.00 to 423.00	100.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water[285])
aniline	394	H	SFG	7	293.16 to 353.16	1.01	L	10.00	Cal.(water at 296.16 K, $2\cdot10^{-9}$ m$^2\cdot$s^{-1})
N,*N*-diphenylamine	394	H	SFG	4	323.16 to 353.16	1.01	scL, L	5.00	Cal.(water at 296.16 K, $2\cdot10^{-9}$ m$^2\cdot$s^{-1})
pyperidine	394	H	SFG	7	293.16 to 353.16	1.01	L	5.00	Cal.(water at 296.16 K, $2\cdot10^{-9}$ m$^2\cdot$s^{-1})
ethylenediamine	393	H	PFG	3	288.00 to 308.00	1.01	L	<5.00	n.a.
formamide	97	H	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
	233	H	PFG-MAS	1	298.16	1.01	L	n.a.	shape (0.9961)

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
formamide-d_2	97	H, D	PFG	3	288.16 to 308.16	1.01	L	1.00	Cal.(heavy water at 298.16 K[40])
N-methylformamide	400	H	SFG	29	278.69 to 313.15	1.00 to 2948.00	L	1.00 *(2.0)*	Cal.(water[40] and benzene[48] at several T)
	306	H	PFG-FT	43	234.50 to 423.00	1.00 to 2000.00	scL, L	2.00 *(5.0)*	Cal.(water at 293 K[40])
N-methylacetamide	306	H	PFG-FT	29	305.50 to 454.00	1.00 to 2000.00	L	2.00 *(5.0)*	Cal.(water at 293 K[40])
n-hexanethiol	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-heptanethiol	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-octanethiol	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
n-dodecanethiol	258	H	PFG	9	278.16 to 358.16	1.01	L	n.a.	Cal.(ethanol[129])
acetic acid	381	H	SFG	4	290.16 to 357.16	1.01	L	5.00 to 10.00	n.a.
	359	H	PFG	1	298.16	1.01	L	3.00	Cal.(water at 298.16 K[326])
	251	H	SSFP	1	room	1.01	L	n.a.	n.a.
acetic acid-*d*	360,361	H	SFG	1	298.16	1.01	L	5.00	shape (1.0874)
octanoic acid	347	H	PFG-FT	2	298.16 and 323.16	1.01	L	n.a.	n.a.
	457	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
nonanoic acid	347	H	PFG-FT	2	298.16, 323.16	1.01	L	n.a.	n.a.
	457	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
decanoic acid	457	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
dodecanoic acid	457	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
tetradecanoic acid	457	H	PFG	3	333.16 to 353.16	1.01	L	n.a.	n.a.
hexadecanoic acid	457	H	PFG	2	343.16 and 353.16	1.01	L	n.a.	n.a.
stearic acid	457	H	PFG	2	343.16 and 353.16	1.01	L	n.a.	n.a.
oleic acid	458	H	PFG-FT	15	293.16 to 363.16	1.01	L	n.a.	n.a.

[a] In the Supporting Information, these values, relative to water, have been converted into absolute ones by taking into account the corresponding self-diffusivities of ref 40. [b] In the original papers, values of benzene-d_6 and pyridine-d_5 were multiplied by the square root of the ratio between the molecular mass of the deuterated species and the hydrogenated species, in order to obtain approximated diffusivities for benzene and pyridine. We have undone this correction in the Supporting Information. [c] Values of 1,2-dimethoxy ethane, diglyme, and triglyme are higher than others reported graphically by the same authors in subsequent papers.[24,459] According to a private communication of K. Hayamizu,[460] the high diffusivities of this ref 387 are less confidable, since they could be affected by convection. 1,2-diethoxyethane and ethyl propionate are suspected to be erroneous too. [d] The nitrobenzene contained 1% H_2O, since the diffusivity of this small amount of water in the solvent was also studied. [e] This chlorobenzene of O'Reilly was erroneous and the correction was given later in the form of an equation,[324] that is cited in Table 6. [f] Tison and Hunt smoothed their experimental measurements taken T_c= 318.70 K and ρ_c= 725 kg·m^{-3}. [g] Zykov et al.[417] affirm that these data of sulfur hexafluoride are more accurate than others previously published by them,[461] and cited in Table 5. [h] Values of saturated H_2O and D_2O of Yoshida et al.[432] were later remeasured and corrected by them in ref 372. [i] This self-diffusion coefficient of Kempka and coworkers is clearly erroneous, since they confirmed it with a point allegedly taken from Kessler et al.[364] which in fact, does not take the value attributed by Kempka.

Table 5. Self-Diffusion Coefficients of Several Substances, Determined by Nuclear Magnetic Resonance, and Reported Graphically

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
methane	226*	H	SFG (constant *G*)	6	94.26 to 111.18	1.01	L	n.a.	Cal.(water at 298.16 K[99])
	226*	H	SFG (constant τ)	7	94.11 to 110.40	1.01	L	n.a.	Cal.(water at 298.16 K[99])
ethane	227*	H	SFG (constant *G*)	14	99.28 to 303.76	Sat	L	n.a.	Cal.(water at 298.16 K[99])
	227*	H	SFG (constant τ)	9	104.27 to 300.29	Sat	L	n.a.	Cal.(water at 298.16 K[99])
	272,273,462[a]	H	SFG	61	286.42 to 333.16	Sat and ρ_c	L,V,G	3.00 to 10.00	Cal.(water at 298.16 K[339])
	463	H	SFG	80	155.00 to 298.00	43.57 to 2361.19	L	n.a.	Cal.(ethane at 298 K[227])
	464	H	SFG	15	91.76 to 271.32	Sat	L	6.00	Cal.(water at 298.16 K[326])
n-pentane	328*	H	SFG	8	190.06 to 297.16	1.01	L	5.00	shape (1.0004?[327])
n-hexane	328*	H	SFG	8	182.28 to 333.89	1.01	L	5.00	shape (1.0004?[327])
	465	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578[319])
	466,467	H	SFG	23	291.92 to 520.07	Sat and ρ_c	L, G	n.a.	shape (1.0309[336])
	468	H	n.a.	5	278.16 to 318.16	1.01	L	n.a.	n.a.
	301,302*	H	PFG-FT	58	253.15 to 368.15	1.00 to 2039.00	L	3.00 to 4.00	Cal.(benzene at 295 and 298.15 K[134])
n-heptane	328*	H	SFG	8	190.28 to 337.61	1.01	L	5.00	shape (1.0004?[327])
	364	H	SFG	13	202.86 to 353.18	1.01	L	n.a.	shape (1.0450)
	467	H	SFG	15	292.70 to 522.24	Sat	L	n.a.	shape (1.0309[336])
	378*	H	SFG	27	185.56 to 373.16	1.01, sat	L	n.a.	shape (0.9830)
n-octane	328*	H	SFG	8	231.80 to 342.62	1.01	L	5.00	shape (1.0004?[327])
	465	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578[319])
	467	H	SFG	16	291.77 to 522.34	Sat	L	n.a.	shape (1.0309[336])
	469	H	SFG, PFG	1	353.16	1.01	L	4.00 to 10.00	shape[470]
	471	H	PFG	8	303.66 to 443.66	1.01, sat	L	n.a.	shape[470,472]
	473	H	PFG	2	328.00 and 338.00	1.01	L	n.a.	shape[470,472]
n-nonane	328*	H	SFG	8	232.47 to 356.15	1.01	L	5.00	shape (1.0004?[327])
	467	H	SFG	14	293.55 to 525.47	Sat	L	n.a.	shape (1.0309[336])
	378*	H	SFG	13	222.06 to 421.96	1.01	L	n.a.	shape (0.9830)
	302*	H	PFG-FT	37	253.15 to 368.15	1.00 to 2000.00	L	4.00	Cal.(benzene at 295 K[134])
n-decane	328*	H	SFG	8	249.22 to 351.10	1.01	L	5.00	shape (1.0004?[327])
	465	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578[319])
	467	H	SFG	15	293.16 to 519.28	Sat	L	n.a.	shape (1.0309[336])
	378*	H	SFG	19	247.86 to 440.16	1.01	L	n.a.	shape (0.9830)
	468	H	n.a.	5	278.16 to 318.16	1.01	L	n.a.	n.a.
	469	H	SFG, PFG	1	353.16	1.01	L	4.00 to 10.00	shape[470]
	471	H	PFG	8	303.66 to 443.66	1.01	L	n.a.	shape[470,472]

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	473	H	PFG	2	328.00 and 338.00	1.01	L	n.a.	shape[470,472]
n-dodecane	465	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578[319])
	378*	H	SFG	10	264.16 to 434.76	1.01	L	n.a.	shape (0.9830)
	468	H	n.a.	5	278.16 to 318.16	1.01	L	n.a.	n.a.
	469	H	SFG, PFG	2	353.16	1.01	L	4.00 to 10.00	shape[470]
	302*	H	PFG-FT	22	268.75 to 368.15	1.00 to 1970.00	L	4.00	Cal.(benzene at 295 K[134])
	471	H	PFG	8	303.66 to 443.66	1.01	L	n.a.	shape[470,472]
	473	H	PFG	1	338.00	1.01	L	n.a.	shape[470,472]
n-tetradecane	465	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578[319])
	378*	H	SFG	11	279.36 to 433.60	1.01	L	n.a.	shape (0.9830)
	468	H	n.a.	5	278.16 to 318.16	1.01	L	n.a.	n.a.
	259	H	PFG-FT	25	293.00 to 443.00	1.01	L	5.00	Cal.(water at 298.16 K[40])
	474	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
n-hexadecane	378*	H	SFG	11	292.68 to 434.26	1.01	L	n.a.	shape (0.9830)
	469	H	SFG, PFG	1	353.16	1.01	L	4.00 to 10.00	shape[470]
	471	H	PFG	8	303.66 to 433.66	1.01	L	n.a.	shape[470,472]
	473	H	PFG	1	338.00	1.01	L	n.a.	shape[470,472]
n-octadecane	328*	H	SFG	12	312.63 to 433.04	1.01	L	5.00	shape (1.0004?[327])
	378*	H	SFG	10	301.86 to 438.76	1.01	L	n.a.	shape (0.9830)
n-nonadecane	474	H	PFG	4	313.16 to 343.16	1.01	L	n.a.	n.a.
n-eicosane	289	H	PFG-FT	5	313.70 to 429.76	Sat	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	471	H	PFG	7	323.16 to 443.66	1.01	L	n.a.	shape[470,472]
	474	H	PFG	5	313.16 to 353.16	1.01	L	n.a.	n.a.
n-tetracosane	469	H	SFG, PFG	1	353.16	1.01	L	4.00 to 10.00	shape[470]
	471	H	PFG	7	323.16 to 443.66	1.01	scL, L	n.a.	shape[470,472]
	474	H	PFG	3	333.16 to 353.16	1.01	L	n.a.	n.a.
n-hexacosane	289	H	PFG-FT	4	333.47 to 428.98	Sat	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	471	H	PFG	6	343.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-octacosane	471	H	PFG	6	343.66 to 443.66	1.01	L	4.00 to 10.00	shape[470,472]
n-triacontane	471	H	PFG	6	343.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-dotriacontane	328*	H	SFG	7	353.06 to 435.08	1.01	L	5.00	shape (1.0004?[327])
	471	H	PFG	6	343.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-hexatriacontane	469	H	SFG, PFG	1	353.16	1.01	L	4.00 to 10.00	shape[470]
	471	H	PFG	5	363.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-tetracontane	289	H	PFG-FT	3	363.22 to 428.69	Sat	L	2.00 *(5.0)*	Cal.(water at 298.16 K[40])
	471	H	PFG	5	363.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-tetratetracontane	471	H	PFG	5	363.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-tetrapentacontane	471	H	PFG	4	383.66 to 443.66	1.01	L	n.a.	shape[470,472]
n-hexacontane	471	H	PFG	4	383.66 to 443.66	1.01	L	n.a.	shape[470,472]

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
neopentane	475	H	SFG	33	256.76 to 307.69	Sat to 689.01	L	5.00 to 10.00	shape
	364*	H	SFG	15	258.70 to 306.40	Sat	L	n.a.	shape (1.0450)
	303	H	SFG	16	267.00 to 450.00	50.00 to 1200.00	L	5.00 *(10.0)*	Cal.(water at (277 to 368) K[285])
isopentane	466	H	SFG	24	271.49 to 468.84	Sat and ρ_c	L, G	n.a.	shape (1.0309[336])
2,2-dimethylbutane	320*	H	SFG	11	212.40 to 311.50	1.01 to 551.58	L	5.00 to 10.00	shape (1.0004?[327])
	304*	H	PFG-FT	34	248.10 to 347.80	1.00 to 2000.00	L	2.00 to 3.00	Cal.(water at several T, P[287])
2,3-dimethylbutane	320*	H	SFG	6	175.48 to 301.56	1.01	L	5.00 to 10.00	shape (1.0004?[327])
2-methylpentane	320*	H	SFG	7	200.00 to 287.50	1.01	L	5.00 to 10.00	shape (1.0004?[327])
3- methylpentane	320*	H	SFG	9	200.00 to 302.00	1.01	L	5.00 to 10.00	shape (1.0004?[327])
ethylene	476	H	SFG	76	263.16 to 313.16	30.40 to 93.92	L,V,G	10.00	shape
	477[b]	H	SFG	59	270.91 to 313.16	140.00 to 360.00 (ρ)	L, G	3.00	shape (1.1091)
	478	H	SFG	29	323.16 to 398.16	70.00 to 563.00 (ρ)	G	6.00	Cal.(supercritical methane[342])
	479	H	SFG	71	273.00 to 348.00	5.63 to 378.27 (ρ)	V, G	0.50 to 1.50	sample location
1-hexene	310	H	PFG	1	313.16	1.01	L	8.00	Cal.(water at several T)
acetylene-d_2	480	D	SFG	31	193.19 to 224.24	Sat	L	n.a.	shape (0.9699[325])
diphenylacetylene	311	H	PFG	9	335.96 to 382.66	1.01	L	n.a.	Cal.(water), theory
cyclopentane	23*	H	SFG, PFG	7	280.92 to 309.37	1.01	L	2.00 to 6.00	shape (0.8986)
cyclohexane	363	H	SFG	12	293.23 to 344.52	1.01	L	< 5.00	shape (1.0450[364])
	274	H	PFG	2	305.16 and 315.16	1.01	L	n.a.	Cal.(water, acetone, benzene, octanol and dodecanol at 298.16 K[334])
	481	H	SFG	10	303.16 to 373.16	Sat	L	n.a.	n.a
	23*	H	SFG, PFG	7	292.33 to 344.10	1.01	L	2.00 to 6.00	shape (0.8986)
	304*	H	PFG-FT	42	295.40 to 393.20	1.00 to 2000.00	L	2.00 to 3.00	Cal.(water at several T, P[287])
	482	H	PFG	12	282.00 to 334.00	1.01	L	n.a.	Cal.(water[369])
cycloheptane	23*	H	SFG, PFG	10	288.66 to 356.75	1.01	L	2.00 to 6.00	shape (0.8986)
cyclooctane	23*	H	SFG, PFG	7	292.57 to 345.90	1.01	L	2.00 to 6.00	shape (0.8986)
	473	H	PFG	2	328.00 and 338.00	1.01	L	n.a.	shape[470,472]
cyclodecane	23*	H	SFG, PFG	7	291.92 to 347.87	1.01	L	2.00 to 6.00	shape (0.8986)
	473	H	PFG	2	328.00 and 338.00	1.01	L	n.a.	shape[470,472]
cyclododecane	23*	H	SFG, PFG	5	342.48 to 382.78	1.01	L	2.00 to 6.00	shape (0.8986)
	473	H	PFG	1	338.00	1.01	L	n.a.	shape[470,472]
cyclohexadecane	473	H	PFG	1	338.00	1.01	L	n.a.	shape[470,472]
cis-perhydroindene	23*	H	SFG, PFG	9	293.46 to 376.86	1.01	L	2.00 to 6.00	shape (0.8986)
cis-decalyn	23*	H	SFG, PFG	7	294.18 to 373.56	1.01	L	2.00 to 6.00	shape (0.8986)
trans-decalyn	23*	H	SFG, PFG	8	296.58 to 377.44	1.01	L	2.00 to 6.00	shape (0.8986)
bicyclohexane	23*	H	SFG, PFG	8	290.76 to 348.49	1.01	L	2.00 to 6.00	shape (0.8986)
perhydrofluorene	23*	H	SFG, PFG	8	285.11 to 362.61	1.01	scL, L	2.00 to 6.00	shape (0.8986)
cis-syn-cis-perhydroanthracene	23*	H	SFG, PFG	8	315.85 to 390.29	1.01	L	2.00 to 6.00	shape (0.8986)
cyclopentene	483*	H	SFG	4	182.16 to 295.66	1.01	L	n.a.	Cal.(water[40] and pentane[320])

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
benzene	318	H	SFG	1	293.16 ?	1.01	L	n.a.	shape (1.0578)
	269	H	SFG (6 cm^2/g)	14	296.19 to 631.01	Sat and beyond	L, G	10.00	shape (1.0173)
	269	H	SFG (180 cm^2/g)	5	298.23 to 580.66	Sat and beyond	L, G	10.00	shape (0.9322)
	362	H	SFG	1	290.16	1.01	L	7.00	n.a.
	363	H	SFG	12	281.26 to 338.98	1.01	L	< 5.00	shape (1.0450[364])
	484	H	SFG	5	300.16 to 373.16	1.01, sat	L	5.00	n.a.
	378*	H	SFG	16	279.06 to 352.16	Sat	L	n.a.	shape (0.9830)
	485	H	n.a.	47	298.16 to 353.16	0.98 to 2353.60	L	5.00 to 6.00	n.a.
	23*	H	PFG	6	294.32 to 341.56	1.01	L	2.00 to 6.00	shape (0.8986)
	23*	H	SFG	8	292.46 to 341.13	1.01	L	2.00 to 6.00	shape (0.8986)
	301*	H	PFG-FT	488	288.15 to 373.15	1.00 to 2000.00	L	3.00	Cal.(benzene at 298.15 K[134])
	304*	H	PFG-FT	25	303.00 to 372.60	1.00 to 2000.00	L	2.00 to 3.00	Cal.(water at several T, P[287])
	266[c]	H	SFG	5	501.41 to 553.61	401.00 (ρ)	biphasic	9.56 to 15.00	shape
	266[c]	H	SFG	4	563.77 to 590.21	401.00 (ρ)	G	9.81 to 15.03	shape
	267	H	SFG	31	289.09 to 561.18	101.00 to 302.00 (ρ)	biphasic	n.a.	shape
	267	H	SFG	44	555.38 to 683.83	101.00 to 302.00 (ρ)	V, G	n.a.	shape
toluene	323*	H	SFG	23	175.09 to 379.21	1.01	scL, L	n.a.	shape (0.9699)
	23	H$_{(CH_3)}$	PFG	8	286.55 to 340.91	1.01	L	2.00 to 6.00	shape (0.8986)
	23	H$_{(ring)}$	PFG	5	286.70 to 331.03	1.01	L	2.00 to 6.00	shape (0.8986)
	486	H	SFG	17	293.16 to 760.16	Sat to 129.44	L, G	n.a.	Cal.(water at 298.16 K[40])
	487	H	SFGSE	23	136.67 to 198.85	1.01	scL, L	n.a.	n.a.
o-xylene	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
m-xylene	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
p-xylene	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
mesitylene	23*	H	SFG, PFG	8	286.03 to 344.13	1.01	L	2.00 to 6.00	shape (0.8986)
1,3,5-triisopropylbenzene	23*	H	SFG, PFG	10	291.33 to 354.25	1.01	L	2.00 to 6.00	shape (0.8986)
o-terphenyl	230	H	PFGSE	5	323.10 to 389.67	1.01	scL, L	n.a.	n.a.
	230	H	SFGSE	26	280.22 to 369.75	1.01	scL, L	n.a.	n.a.
$\alpha\alpha\beta$-trinaphthylbenzene	488	H	SFGSE	9	405.16 to 476.16	1.01	scL, L	n.a.	n.a.
1,2-dimethoxyethane	459	H	PFG	1	303.16	1.01	L	n.a.	n.a.
diglycole dimethyl ether	24	H	PFG	6	303.16 to 353.16	1.01	L	n.a.	shape (1.0000)
	489	H	PFG	15	233.16 to 373.16	1.01	L	n.a.	shape
triglyme	24	H	PFG	6	303.16 to 353.16	1.01	L	n.a.	shape (1.0000)
tetraglyme	24	H	PFG	6	303.16 to 353.16	1.01	L	n.a.	shape (1.0000)
pentaglyme	24	H	PFG	6	303.16 to 353.16	1.01	L	n.a.	shape (1.0000)
tetramethoxymethane	426*	H	SFG	8	280.60 to 347.24	1.01	L	2.00 to 10.00	shape (0.9221)
furan	490	H	SFG	9	295.45 to 402.91	Sat	L	5.00	n.a.
dioxane	491	H	SFG	2	307.16 and 327.16	1.01	L	n.a.	Cal.(water at 298.16 K[339])
	316	H	SFG?	1	293.16	1.01	L	n.a.	shape (1.0578)

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	426*	H	SFG	6	296.53 to 337.75	1.01	L	2.00 to 10.00	shape (0.9221)
trioxane	426*	H	SFG	4	342.24 to 367.34	1.01	L	2.00 to 10.00	shape (0.9221)
12-crown-4	426*	H	SFG	5	294.17 to 351.45	1.01	L	2.00 to 10.00	shape (0.9221)
15-crown-5	426*	H	SFG	12	298.25 to 375.68	1.01	L	2.00 to 10.00	shape (0.9221)
18-crown-6	426*	H	SFG	11	315.92 to 369.93	1.01	L	2.00 to 10.00	shape (0.9221)
acetone	362	H	SFG	1	293.16	1.01	L	7.00	n.a.
	316	H	SFG?	1	293.16	1.01	L	n.a.	shape (1.0578)
	378*	H	SFG	12	182.86 to 331.16	1.01, sat	L	n.a.	shape (0.9830)
	492	H	SFG	8	275.16 to 343.16	1.01, sat	L	n.a.	shape (0.9543)
diethyl carbonate	459	H	PFG	1	303.16	1.01	L	n.a.	n.a.
propylene carbonate	493	H	PFG	1	295.16	1.01	L	n.a.	Cal.(water[285])
	494	H	SFGSE	32	178.88 to 320.34	1.01	scL, L	n.a.	n.a.
	459	H	PFG	1	303.16	1.01	L	n.a.	n.a.
phenolphthalein dimethyl ether	495	H	SFGSE	8	343.03 to 403.00	1.01	scL, L	n.a.	n.a.
	488	H	SFGSE	23	337.03 to 427.20	1.01	scL, L	n.a.	n.a.
cresolphthalein dimethyl ether	488	H	SFGSE	15	370.58 to 430.59	1.01	scL, L	n.a.	n.a.
pyridine	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
	396*	H	SFG	18	253.02 to 388.18	1.01	L	n.a.	shape (0.9699)
α-picoline	316	H	SFG?	1	293.16	1.01	L	n.a.	shape (1.0578)
tert-butyl nitrile	303	H	SFG	19	300.00 to 464.00	50.00 to 1500.00	L	5.00 *(10.0)*	Cal.(water at (277 to 368) K[285])
2-nitroisobutane	364*	H	SFG	17	212.88 to 330.88	1.01	L	n.a.	shape (1.0450)
2,2-dinitropropane	496[d]	H	PFG	8	323.66 to 357.16	1.01	scL, L	10.00	n.a.
nitrobenzene	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
triethyl amine	362	H	SFG	1	290.16	1.01	L	7.00	n.a.
dimethyl aniline	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
cis-*N*-isopropyl-*N*-methylacetamide	305	H	PFG-FT	4	241.64 to 297.93	1.01	L	2.00 *(5.0)*	Cal.(water at 293 K[40])
trans-*N*-isopropyl-*N*-methylacetamide	305	H	PFG-FT	4	241.64 to 297.93	1.01	L	2.00 *(5.0)*	Cal.(water at 293 K[40])
thiophene	484	H	SFG	5	300.16 to 373.16	1.01, sat	L	5.00	n.a.
	497	H	SFG	13	302.80 to 574.62	Sat	L	5.00	n.a.
dimethylsulfoxide	498	H	PFG	3	288.20 to 308.20	1.01	scL, L	3.00 *(5.0)*	n.a.
tri-*n*-butyl phosphate	348	H, ^{31}P	SFG	20	227.94 to 344.10	1.01	L	5.00 to 10.00	n.a.
tetramethyl silane	475*	H	SFG	20	191.74 to 300.95	Sat to 688.69	L	5.00 to 10.00	shape
	364*	H	SFG	18	212.64 to 299.37	1.01	L	n.a.	shape (1.0450)
	302*	H	PFG-FT	52	253.15 to 368.15	1.00 to 2000.00	L	4.00	Cal.(benzene at 295 K[134])
tetrametoxy silane	364*	H	SFG	17	272.92 to 372.90	1.01	L	n.a.	shape (1.0450)
	426*	H	SFG	8	283.30 to 340.53	1.01	L	2.00 to 10.00	shape (0.9221)
tetraisopropoxy silane	426*	H	SFG	6	288.07 to 353.05	1.01	L	2.00 to 10.00	shape (0.9221)

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
hexamethyldisiloxane	499*	H	SFG	11	272.46 to 338.66	1.01 to 665.05	L	5.00 to 10.00	shape
octamethyltrisiloxane	499*	H	SFG	11	272.16 to 338.66	1.01 to 683.94	L	5.00 to 10.00	shape
decamethyltetrasiloxane	499*	H	SFG	11	272.16 to 338.66	1.01 to 683.94	L	5.00 to 10.00	shape
dodecamethylpentasiloxane	499*	H	SFG	10	272.16 to 338.66	1.01 to 641.45	L	5.00 to 10.00	shape
tetradecamethylhexasiloxane	499*	H	SFG	11	272.96 to 338.66	1.01 to 683.94	L	5.00 to 10.00	shape
hexadecamethylheptasiloxane	499*	H	SFG	13	272.46 to 338.66	1.01 to 686.10	L	5.00 to 10.00	shape
eicosamethylnonasiloxane	499*	H	SFG	22	238.16 to 338.66	1.01 to 675.84	L	5.00 to 10.00	shape
hexamethylcyclotrixilosane	23*	H	SFG, PFG	6	340.91 to 393.68	1.01	L	2.00 to 6.00	shape (0.8986)
octamethylcyclotetrasiloxane	426*	H	SFG	6	294.22 to 349.16	1.01	L	2.00 to 10.00	shape (0.9221)
	23*	H	SFG, PFG	7	293.80 to 345.49	1.01	L	2.00 to 6.00	shape (0.8986)
	296	H	PFG-FT	43	289.00 to 438.00	1.00 to 2000.00	scL, L	5.00	Cal.(water at 298.16 K[40])
decamethylcyclopentasiloxane	23*	H	SFG, PFG	7	294.67 to 345.86	1.01	L	2.00 to 6.00	shape (0.8986)
hexamethylcyclotrisilazane	296	H	PFG-FT	76	209.00 to 490.00	1.00 to 2000.00	scL, L	5.00	Cal.(water at 298.16 K[40])
tetramethyl germane	364*	H	SFG	18	222.89 to 311.16	1.01	L	n.a.	shape (1.0450)
tetramethoxy germane	364*	H	SFG	13	264.60 to 383.43	1.01	L	n.a.	shape (1.0450)
	426*	H	SFG	8	280.60 to 342.93	1.01	L	2.00 to 10.00	shape (0.9221)
tetra-*tert*-butoxy germane	426*	H	SFG	7	292.56 to 360.98	1.01	L	2.00 to 10.00	shape (0.9221)
tetramethyl tin	364*	H	SFG	25	241.75 to 329.49	1.01	L	n.a.	shape (1.0450)
	426*	H	SFG	5	273.13 to 303.82	1.01	L	2.00 to 10.00	shape (0.9221)
tetraoctyl tin	426*	H	SFG	13	297.21 to 359.74	1.01	L	2.00 to 10.00	shape (0.9221)
tetramethyl lead	364*	H	SFG	18	249.33 to 324.40	1.01	L	n.a.	shape (1.0450)
tetra-*tert*-butoxy titanium	426*	H	SFG	8	290.79 to 364.83	1.01	L	2.00 to 10.00	shape (0.9221)
dichloromethane	500*	H	SFG	29	280.66 to 326.76	Sat	L	n.a.	Cal.(water at 298.16 K[339])
	396*	n.a.	SFG	14	195.38 to 321.97	1.01, sat	L	n.a.	shape (0.9699)
chloroform	362	H	SFG	1	290.16	1.01	L	7.00	n.a.
	501*	H	SFG	36	274.21 to 332.63	1.01	L	3.00 to 5.00	n.a.
chlorodifluoromethane	297	n.a.	PFG	58	147.50 to 385.50	1.00 to 2000.00	L, G	5.00	Cal.(water at 298.16 K[40])
trichlorofluoromethane	502	^{19}F	SFG	8	164.20 to 422.34	Sat	L	n.a.	shape
	468	^{19}F	n.a.	5	278.16 to 318.16	Sat	L	n.a.	n.a.
dibromomethane	500*	H	SFG	42	285.60 to 353.31	1.01	L	n.a.	Cal.(water at 298.16 K[339])
	503*	H	PFG	8	286.16 to 364.66	1.01	L	10.00	n.a.
tribromomethane	501*	H	SFG	34	277.51 to 347.85	1.01	scL, L	3.00 to 5.00	n.a.
iodomethane	504[e]	H	SFG	6	302.16	0.98 to 6853.56	L	n.a.	not evaluated (relative values only)
	501*	H	SFG	31	271.16 to 314.88	1.01	L	3.00 to 5.00	n.a.
diiodomethane	500*	H	SFG	39	283.53 to 350.97	1.01	L	n.a.	Cal.(water at 298.16 K[339])
1,2-dichloroethane	505	H	SFG	8	294.72 to 436.04	Sat	L	5.00	n.a.
1,1,1-trichloroethane	496	H	SFG	8	236.16 to 287.66	1.01	scL, L	10.00	n.a.
1,2-dibromotetrafluoroethane	304*	^{19}F	PFG-FT	52	247.70 to 372.00	1.00 to 2000.00	L	2.00 to 3.00	Cal.(water at several T, P[287])
1,2-dibromoethane	311	H	PFG	9	303.16 to 385.16	1.01	L	n.a.	Cal.(water), theory

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	503*	H	PFG	11	286.16 to 401.16	1.01	L	10.00	n.a.
1,8-dibromooctane	503*	H	PFG	11	295.16 to 417.16	1.01	L	10.00	n.a.
1,10-dibromodecane	311	H	PFG	7	312.80 to 385.35	1.01	L	n.a.	Cal.(water), theory
	503*	H	PFG	10	303.16 to 417.16	1.01	L	10.00	n.a.
1,12-dibromododecane	503*	H	PFG	9	313.16 to 417.16	1.01	L	10.00	n.a.
tert-butyl chloride	364*	H	SFG	9	249.84 to 316.14	1.01	L	n.a.	shape (1.0450)
	506[f]	H	SFG	57	245.58 to 507.68	Sat and beyond	scL, L,G	n.a.	shape (0.9699)
	496	H	PFG	8	242.16 to 287.66	1.01	scL, L	10.00	n.a.
tert-butyl bromide	364*	H	SFG	11	260.70 to 330.30	1.01	L	n.a.	shape (1.0450)
tert-butyl iodide	364*	H	SFG	12	240.31 to 344.01	1.01	L	n.a.	shape (1.0450)
perfluorodecalin	23*	H, ^{19}F	SFG, PFG	7	291.10 to 347.81	1.01	L	2.00 to 6.00	shape (0.8986)
fluorobenzene	378*	H	SFG	18	234.96 to 356.16	1.01	L	n.a.	shape (0.9830)
hexafluorobenzene	363*	^{19}F	SFG	11	292.80 to 341.86	1.01	L	< 5.00	shape (1.0450[364])
	507*	^{19}F	SFG	101	288.16 to 423.16	Sat to 1920.80	L	6.00 to 8.00	shape (1.0000[286])
	469	^{19}F	SFG, PFG	1	353.16	1.01	L	4.00 to 10.00	shape[470]
	23*	^{19}F	SFG, PFG	8	286.96 to 339.11	1.01	L	2.00 to 6.00	shape (0.8986)
chlorobenzene	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
	378*	H	SFG	15	229.56 to 410.46	1.01, sat	L	n.a.	shape (0.9830)
bromobenzene	378*	H	SFG	15	241.26 to 429.36	1.01	scL, L	n.a.	shape (0.9830)
iodobenzene	378*	H	SFG	18	242.66 to 445.36	1.01	L	n.a.	shape (0.9830)
trifluoromethylbenzene	409	H	SFG	13	283.16 to 371.16	1.01	L	5.00	n.a.
perfluorobenzonitrile	304*	^{19}F	PFG-FT	50	299.00 to 398.20	1.00 to 2000.00	L	2.00 to 3.00	Cal.(water at several T, P[287])
dinitrofluoromethane	409	H	SFG	4	298.16 to 353.16	1.01	L	5.00	n.a.
1-fluoro-1,1-dinitroethane	409	H	SFG	7	288.16 to 363.16	1.01	L	5.00	n.a.
trinitrofluoromethane	409	^{19}F	SFG	6	293.16 to 353.16	1.01	L	5.00	n.a.
trimethylfluorosilane	364*	H	SFG	18	199.23 to 293.72	1.01, sat	L	n.a.	shape (1.0450)
trimethylchlorosilane	364*	H	SFG	16	219.84 to 316.45	1.01	L	n.a.	shape (1.0450)
trichloro (3,3,3-trifluoropropyl) silane	409	H	SFG	5	298.16 to 368.16	1.01	L	5.00	n.a.
trichloro (1-chloro-3,3,3-trifluoropropyl) silane	409	H	SFG	5	298.16 to 371.16	1.01	L	5.00	n.a.
trimethylbromosilane	364*	H	SFG	14	231.08 to 330.23	1.01	L	n.a.	shape (1.0450)
krypton	508	^{83}Kr	SFG	40	115.35 to 212.93	Sat and beyond	L, G	n.a.	shape
xenon	420*	^{129}Xe	SFG	19	166.65 to 233.25	10.13 and 20.27	L	n.a.	shape (1.0569)
	270[g]	^{129}Xe	SFG	82	177.32 to 289.26	Sat, 495.51 (ρ)	L,V,G	5.00 to 8.30	Cal.(water at 298.16 K, 2.39·10^{-9} m^2·s^{-1})
nitrogen-$^{15}N_2$	509*	^{15}N	SFG	9	77.47 to 93.01	Sat	L	10.00	shape
fluorine	510	^{19}F	SFG	6	56.52 to 96.22	Sat	L	n.a.	Cal.(water[339]), shape (0.9699?[324])
carbon-^{13}C monoxide	511	^{13}C	SFG – FT	8	69.16 to 103.16	Sat, 1730.00	L	10 at *sat*, 20 at P	shape
carbon-^{13}C dioxide	512[h]	^{13}C	SFG(set 1)	38	217.94 to 304.90	Sat, 468.00 (ρ)	L, G	10.00	shape

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	512[h]	^{13}C	SFG(set 2)	28	219.39 to 306.48	Sat, 468.00 (ρ)	L, G	<10.00	shape
sulfur hexafluoride	477[i]	^{19}F	SFG	57	313.37 to 333.07	250.00 to 880.00 (ρ)	V, G	3.00	shape (1.1091)
	513[e]	^{19}F	SFG	47	317.26 to 319.56	724.00 to 794.00 (ρ)	L, G	6.00	not evaluated (relative values only)
	461	^{19}F	SFG	32	300.00 to 360.00	65.78 to 508.97 (ρ)	V, G	4.00	n.a.
normal hydrogen	514*	H	SFG	26	14.56 to 20.51	Sat	L	6.00	shape
	515	H	SFG	39	20.44 to 55.53	< 78.64 (ρ)	L,V,G	10.00	shape
	516*	H	SFG	14	14.01 to 22.50	Sat	L	10.00	shape (0.9699)
20% *o*-H_2 and 80% *p*-H_2	515	*o*-H	SFG	1	35.88	< 40.47 (ρ)	G	10.00	shape
22.2% *o*-H_2 and 77.8% *p*-H_2	515	*o*-H	SFG	6	25.60	66.89 to 73.32 (ρ)	L	10.00	shape
25% *o*-H_2 and 75% *p*-H_2	515	*o*-H	SFG	1	45.00	< 40.47 (ρ)	G	10.00	shape
37.5% *o*-H_2 and 62.5% *p*-H_2	515	*o*-H	SFG	1	20.17	< 40.47 (ρ)	V	10.00	shape
31% *o*-H_2 and 69% *p*-H_2	515	*o*-H	SFG	3	35.85 to 55.50	< 40.47 (ρ)	G	10.00	shape
50% *o*-H_2 and 50% *p*-H_2	515	*o*-H	SFG	2	36.09 and 44.88	< 40.47 (ρ)	G	10.00	shape
deuterium	516*	D	SFG	14	18.19 to 24.02	Sat	L	10.00	shape (0.9699)
helium 3	100	^{3}He	SFG	52	0.45 to 4.20	2.43 to 67.89	L,G	2.00	sample location, shape
	517[j]	^{3}He	SFG	67	0.07 to 2.97	0.06 to 0.08, sat	L	5.00	theory
	518[k]	^{3}He	SFG	39	0.03 to 0.14	0.07 to 0.12	L	n.a.	theory
	519[k]	^{3}He	SFG	18	0.02 to 0.08	0.16	L	7.00	theory
	520[k]	^{3}He	SFG	76	0.02 to 0.29	0.86 to 28.57	L	3.00	theory + correction
	335	^{3}He	SFG	25	1.72 to 4.24	< 124.63 (ρ)	V, G	< 6.00	theory, shape
	521	^{3}He	SFG	35	3.00 to 4.23	< 78.66 (ρ)	V, G	5.00	n.a.
	268	^{3}He	SFG (2.5 mm)	2	1.36 and 1.95	Sat	L	n.a.	shape
	268	^{3}He	SFG (3 mm)	1	2.50	Sat	L	n.a.	shape
	268	^{3}He	SFG (8 mm)	7	1.39 to 2.74	Sat	L	n.a.	shape
	268	^{3}He	SFG (10 mm)	3	1.37 to 2.65	Sat	L	n.a.	shape
neon (enriched to 51% in ^{21}Ne)	522*	^{21}Ne	SFG	10	25.21 to 33.15	Sat	L	10.00	theory, shape
water	504[e]	H	SFG	7	301.96	0.98 to 9191.19	L	n.a.	not evaluated (relative values only)
	327	H	SFG	1	298.66	1.01	L	n.a.	n.a.
	269	H	SFG (6 cm^2/g)	19	298.21 to 651.61	Sat and beyond	L, G	10.00	shape (1.0173)
	269	H	SFG (80 cm^2/g)	16	300.00 to 651.61	Sat and beyond	L, G	10.00	shape (0.9322)
	523	H	SFG	5	298.16 to 353.16	Sat	L	4.00	n.a.
	523	H	PFG	6	298.16 to 413.16	Sat	L	4.00	n.a.
	364	H	SFG	7	295.16 to 353.16	1.01	L	n.a.	shape (1.0450)
	491	H	SFG	3	283.16 to 327.16	1.01	L	n.a.	Cal.(water at 298.16 K[339])
	524	H	SFG	14	278.16 to 343.16	1.01	L	n.a.	shape
	477	H	SFG	1	298.16	1.01	L	0.78	shape (1.1091)
	498	H	PFG	3	288.20 to 308.20	1.01	L	3.00 *(5.0)*	n.a.
	525	H	PFG	15	268.16 to 393.16	Sat	scL, L	n.a.	n.a.

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
	378*	H	SFG	12	273.89 to 371.34	1.01	L	n.a.	shape (0.9830)
	526	H	SFG	121	277.16 to 333.16	1.01 to 7599.38	L	n.a.	shape
	527	H	SFG	34	253.06 to 275.36	474.76 to 2279.27	scL, L	3.00 to 6.00	Cal.(water at several T, P[40,202,209])
	528	H	SFG	10	298.16	1.00 to 4500.00	L	5.00	Cal.(water at 298.16 K[40])
	23	H	PFG	11	284.07 to 349.71	1.01	L	2.00 to 6.00	shape (0.8986)
	23	H	SFG	11	295.97 to 349.91	1.01	L	2.00 to 6.00	shape (0.8986)
	492	H	SFG	8	275.16 to 343.16	1.01	L	n.a.	shape (0.9543)
	304	H	PFG-FT	27	280.60 to 333.20	1.00 to 2000.00	L	2.00 to 3.00	Cal.(water at several T, P[287])
	249	H	QUEST	48	292.16 to 319.06	1.01	L	0.65 to 2.37	n.a.
	529	H	PFG	11	278.16 to 329.16	1.01	L	1.00	Cal.(water at 298.16 K[40])
heavy water	529	D	PFG	10	280.16 to 328.16	1.01	L	< 1.00	Cal.(water at 298.16 K[40])
ammonia	325*	H	SFG	25	197.04 to 297.74	Sat	L	n.a.	shape (0.9699)
	529	H	PFG	7	273.16 to 303.16	Sat	L	< 1.00	Cal.(water at 298.16 K[40])
ammonia-d_3	325*	D	SFG	30	200.08 to 290.16	Sat	L	n.a.	shape (0.9699)
	529	H	PFG	5	278.16 to 298.16	Sat	L	< 1.00	Cal.(water at 298.16 K[40])
hydrogen fluoride	322*,[l]	^{19}F	SFG	12	193.16 to 296.16	Sat	L	n.a.	Cal.(water[339]), shape (0.9699?[324])
	322*,[l]	H	SFG	12	193.16 to 295.66	Sat	L	n.a.	Cal.(water[339]), shape (0.9699?[324])
hydrogen chloride	322*	H	SFG	11	163.16 to 253.16	Sat	L	n.a.	Cal.(water[339]), shape (0.9699?[324])
	442	H	SFG(set 1)	14	163.61 to 306.02	Sat	L	n.a.	shape
	442	H	SFG(set 2)	13	298.16 to 331.66	Sat and ρ_c	L, G	n.a.	shape
deuterium chloride	442	D	SFG	15	160.02 to 307.44	Sat	L	n.a.	shape
methanol	319	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578)
	317	H	SFG	1	293.16	1.01	L	n.a.	n.a.
	501*	H	SFG	51	271.69 to 349.36	Sat	L	3.00 to 5.00	n.a.
	530	H	PFG-FT	1	305.16	1.01	L	n.a.	Cal.(water at 305.16 K[40])
methanol-*d*	531	H	SFG	7	293.16 to 363.16	Sat	L	5.00 to 6.00	n.a.
ethanol	319	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578)
	317	H	SFG	1	293.16	1.01	L	n.a.	n.a.
	532*, [m]	H	PFG	41	287.80 to 317.80	1.00 to 1525.00	L	n.a.	Cal.(water[40] and benzene[48])
1-propanol	319	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578)
	317	H	SFG	1	293.16	1.01	L	n.a.	n.a.
	532*, [m]	H	PFG	45	287.80 to 317.80	1.00 to 3600.00	L	n.a.	Cal.(water[40] and benzene[48])
2-propanol	319	H	SFG	1	293.16	1.01	L	n.a.	shape (1.0578)
1-butanol	317	H	SFG	1	293.16	1.01	L	n.a.	n.a.
tert-butanol	364*	H	SFG	13	293.73 to 353.11	1.01	L	n.a.	shape (1.0450)
tert-butanol-*d*	303	n.a.	SFG	25	303.00 to 476.00	50.00 to 1200.00	L	5.00 *(10.0)*	Cal.(water at (277 to 368) K[285])
1-octanol	533	H	PFG	8	288.16 to 353.16	1.01	L	n.a.	n.a.
oleyl alcohol	534	H	PFG	8	303.16 to 373.16	1.01	L	n.a.	n.a.
phenyl salicylate	488	H	SFGSE	24	248.64 to 368.44	1.01	scL, L	n.a.	n.a.

substance	ref	atom	method	points	*T*/ K	*P*/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
glycerol	535	H	PFG	24	288.27 to 438.42	1.01	scL, L	< 12.00	Cal.(water at 298.2 K[425])
	536	H	n.a.	2	283.16 and 373.16	1.01	scL, L	n.a.	n.a.
	537	H	PFG	5	299.16 to 323.16	1.01	L	20.00	n.a.
	537	H	SFG	5	329.16 to 354.16	1.01	L	5.00	n.a.
	488	H	SFGSE	39	255.71 to 457.69	1.01	scL, L	n.a.	n.a.
N- (5-nitropyridyl)-2-*L*-prolinol	28	H	PFG (Δ=40,*G*=239)	7	332.98 to 369.28	1.01	scL, L	n.a.	n.a.
	28	H	PFG (Δ=20,*G*=277)	5	346.94 to 366.92	1.01	scL, L	n.a.	n.a.
	28	H	PFG (Δ=20,*G*=239)	8	334.14 to 361.90	1.01	scL, L	n.a.	n.a.
aniline-*N*,*N*-d_2-2,4,6-d_3	274	n.a.	PFG	2	305.16 and 315.16	1.01	L	n.a.	Cal.(water, acetone. benzene, octanol and dodecanol at 298.16 K[334])
m-fluoroaniline	538*	H	SFGSE	15	203.40 to 382.25	1.01	scL, L	n.a.	n.a.
pyperidine	484	H	SFG	5	300.16 to 373.16	1.01	L	5.00	n.a.
2-cyclooctylamino-5-nitropyridine	28*	H	PFG (Δ=15,*G*=261)	13	323.46 to 402.06	1.01	scL, L	n.a.	n.a.
	28*	H	PFG (Δ=10,*G*=276)	7	323.77 to 357.39	1.01	scL, L	n.a.	n.a.
2-(α-methylbenzylamino)-5-nitropyridine	28*	H	PFG (Δ=10,*G*=268)	10	339.41 to 403.01	1.01	scL, L	n.a.	n.a.
	28*	H	PFG (Δ=15,*G*=268)	2	334.47 and 339.41	1.01	scL	n.a.	n.a.
cis-*N*-methylformamide	539	H	PFG-FT	20	258.00 to 322.47	1.00 to 2000.00	scL, L	2.00 *(5.0)*	Cal.(water at 293 K[40])
trans-*N*-methylformamide	539	H	PFG-FT	20	258.00 to 322.47	1.00 to 2000.00	scL, L	2.00 *(5.0)*	Cal.(water at 293 K[40])
acetic acid	317	H	SFG	1	293.16	1.01	L	n.a.	n.a.
	530	H	PFG-FT	1	305.16	1.01	L	n.a.	Cal.(water at 305.16 K[40])
	23*	H	SFG, PFG	6	293.99 to 344.71	1.01	L	2.00 to 6.00	shape (0.8986)
acetic acid-*d*	378*	H	SFG	8	290.26 to 389.26	1.01	L	n.a.	shape (0.9830)
pivalic acid	23*	H	SFG, PFG	7	306.71 to 346.56	1.01	scL, L	2.00 to 6.00	shape (0.8986)
octanoic acid	533	H	PFG	8	288.16 to 353.16	1.01	scL, L	n.a.	n.a.
decanoic acid	474	H	PFG	6	323.16 to 353.16	1.01	L	n.a.	n.a.
dodecanoic acid	540	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
	474	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.
stearic acid	541	H	PFG	5	343.16 to 373.16	1.01	L	n.a.	n.a.
	474	H	PFG	2	348.16 and 353.16	1.01	L	n.a.	n.a.
	29	H	PFG	9	353.16 to 393.16	1.01	L	8.00	Cal.(water at several *T*)
petroselinic acid	541	H	PFG	8	308.16 to 373.16	1.01	L	n.a.	n.a.
oleic acid	534	H	PFG	15	293.16 to 363.16	1.01	L	n.a.	n.a.
	541	H	PFG	9	298.16 to 373.16	1.01	L	n.a.	n.a.
	371	H	PFG	6	303.16 to 353.16	1.01	L	8.00	n.a.
	29	H	PFG	10	303.16 to 393.16	1.01	L	8.00	Cal.(water at several *T*)
asclepic acid	541	H	PFG	9	298.16 to 373.16	1.01	L	n.a.	n.a.
eleaidic acid	541	H	PFG	6	323.16 to 373.16	1.01	L	n.a.	n.a.
	29	H	PFG	14	328.16 to 393.16	1.01	L	8.00	Cal.(water at several *T*)
hydrocinnamic acid	540	H	PFG	4	323.16 to 353.16	1.01	L	n.a.	n.a.

substance	ref	atom	method	points	T/ K	P/bar or ρ/(kg·m^{-3})	state	% error	gradient evaluation
trifluoroacetic acid	23	H, ^{19}F	SFG, PFG	6	293.53 to 346.37	1.01, sat	L	2.00 to 6.00	shape (0.8986)
heptadecafluorinated oleic acid [n]	29	H	PFG	10	303.16 to 393.16	1.01	L	8.00	Cal.(water at several T)
heptadecafluorinated elaidic acid[n]	29	H	PFG	7	333.16 to 393.16	1.01	L	8.00	Cal.(water at several T)
heptadecafluorinated stearic acid[n]	29	H	PFG	7	363.16 to 393.16	1.01	L	8.00	Cal.(water at several T)

[a] The critical temperature of this ethane doped with 1% O_2 decreased to 305.08 K, but nothing is said about the critical density. [b] The critical properties of this ethylene were (282.56±0.05) K, (50.66±0.10) bar and (210±5) kg·m^{-3}. [c] The critical temperature of this benzene was 563.16 K. [d] The melting point of this 2,2-nitropropane seems appears to be between 326.66 and 327.66 K, a range slightly higher than that found in several databases. [e] In the Supporting Information, the relative diffusivities of iodomethane and water of Benedek and Purcell[504] has been converted into absolute ones by taking into account the diffusivities of Mills[40] and Sandhu[501] around 302 K. The same was done with the values of Zykov et al.,[513] which were relatives to the critical diffusivity of sulfur hexafluoride (took as 29.2·10^{-9} m^2·s^{-1} from Tison and Hunt,[415] and in good agreement with a subsequent work of Zykov.[417]). [f] O'Reilly said that the critical temperature of the *tert*-butyl chloride is 490 K, but all the databases consulted gave a T_c of around 507 K. [g] The critical properties of this xenon, doped with 0.5% O_2, are 289.174±0.003 K and 1097.19 kg·m^{-3}. [h] The critical properties of this $^{13}CO_2$ were (304.16 ±0.05) K and 468 kg·m^{-3}. [i] The critical properties for this SF_6 were (318.72±0.05) K, (37.59±0.10) bar and (730±20) kg·m^{-3}. [j] According to Anderson et al.,[520] the work of Hart has inaccuracies in the temperature scale. [k] Anderson and coworkers measured self-diffusion coefficients of helium 3 three times,[518-520] but considered that in the first case[518] there were systematic errors. [l] O'Reilly remeasured the self-diffusivities of hydrogen fluoride and reported them later in the form of an equation,[441] which is compiled in Table 6. [m] Ethanol and propanol of Meckl and Zeidler are given in figures of $\mathfrak{D}_{11}$ vs ρ. Fortunately, the paper also provided equations of state that allows us to determine the values of the pressure. [n] The full names of these semi-fluorinated fatty acids were 11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-heptadecafluoro-oleic acid, 11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-heptadecafluoro-eleaidic acid and 11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-heptadecafluoro-stearic acid.

Table 6. Self-Diffusion Coefficients of Several Substances, Determined by Nuclear Magnetic Resonance, and Reported in the Form of Mathematical Equations

substance	ref	T/ K	P/ bar	$10^9 \cdot \mathbb{D}/(m^2 \cdot s^{-1})$	$E_{\mathfrak{D}}/$ (kcal·mol^{-1})	$V_{\mathfrak{D}}/$ (cm^3·mol^{-1})	$10^9 \cdot \mathfrak{D}_{11}/(m^2 \cdot s^{-1})$	% error	gradient evaluation
n-pentane	320,328[a]	190.06 to 297.16	< 551.57 ?	n.a.	1.54 ± 0.07	11.4	5.45 (298.16 K)	5.00	shape (1.0004?[327])
	542[a]	n.a.	1.01 to 689.0	n.a.	n.a.	17.0, 18.0	n.a.	5.88, 5.56	shape (1.0004?[327])
n-hexane	320,328	182.28 to 333.89	< 551.57 ?	n.a.	2.07 ± 0.13	16.8	4.21 (298.16 K)	5.00	shape (1.0004?[327])
n-heptane	320,328	190.28 to 337.61	< 551.57 ?	n.a.	2.19 ± 0.06	20.0	3.12 (298.16 K)	5.00	shape (1.0004?[327])
n-octane	320,328	231.80 to 342.62	< 551.57 ?	n.a.	2.42 ± 0.18	16.7	2.00 (298.16 K)	5.00	shape (1.0004?[327])
n-nonane	320,328	232.47 to 356.15	< 551.57 ?	n.a.	3.08 ± 0.10	21.8	1.70 (298.16 K)	5.00	shape (1.0004?[327])
n-decane	320,328	249.22 to 351.10	< 551.57 ?	n.a.	3.56 ± 0.09	21.6	1.31 (298.16 K)	5.00	shape (1.0004?[327])
n-dooctacontane	334	n.a.	1.01 or sat.	n.a.	7.00	n.a.	0.11 (393.16 K)	n.a.	shape
n-tetranonacontane	334	n.a.	1.01 or sat.	n.a.	6.50	n.a.	0.055 (393.16 K)	n.a.	shape
neopentane	331	n.a.	1.01 or sat.	420	2.64	n.a.	4.86 (298.16 K)	5.00 to 10.00	Cal.(water[339])? shape?
isopentane	331,334	n.a.	< 709.23	100	1.73	34.0	5.30 (298.16 K)	5.00 to 10.00	Cal.(water[339])? shape?
2-methylpentane	320	200.00 to 287.50	< 551.57 ?	n.a.	1.86 ± 0.10	16.5	3.98 (298.16 K)	5.00	shape (1.0004?[327])
3-methylpentane	320	200.00 to 302.00	< 551.57 ?	n.a.	1.94 ± 0.11	16.5	3.61 (298.16 K)	5.00	shape (1.0004?[327])
2,2-dimethylbutane	320	212.40 to 311.50	< 551.57 ?	n.a.	2.70 ± 0.04	27.2	3.41 (298.16 K)	5.00	shape (1.0004?[327])
2,3-dimethylbutane	320	175.48 to 301.56	< 551.57 ?	n.a.	2.00 ± 0.03	15.9	3.50 (298.16 K)	5.00	shape (1.0004?[327])
cyclohexane	331,334	n.a.	<709.23	3000	4.56	28.0	1.38 (298.16 K)	5.00 to 10.00	Cal.(water[339])? shape?
	543	290 to 360	1.01, sat.	370 ± 120	3.33 ± 0.30	n.a.	n.a.	n.a.	shape
	276[b]	298.16 to 363.16	Sat	n.a.	3.34	n.a.	1.74 (303.16 K)	<5.00	n.a.
cyclooctatetraene	334	n.a.	1.01 or sat.	n.a.	3.60	n.a.	0.70 (298.16 K)	n.a.	shape
benzene	331,334	n.a.	<709.23	60	2.00	20.0	2.14 (298.16 K)	5.00 to 10.00	Cal.(water[339])? shape?
	276[b]	263.66 to 373.16	Sat.	n.a.	3.20	n.a.	2.02 (293.16 K)	<5.00	n.a.
toluene	276[b]	298.16 to 363.16	1.01	n.a.	2.67	n.a.	2.59 (303.16 K)	<5.00	n.a.
m-xylene	276	n.a.	1.01 or sat.	n.a.	2.58	n.a.	2.56 (313.16 K)	<5.00	n.a.
p-xylene	276	n.a.	1.01 or sat.	n.a.	2.86	n.a.	2.75 (313.16 K)	<5.00	n.a.
mesitylene	304[c]	247.00 to 373.80	1.00 to 2000	147.53	2.669 $-1.05 \cdot 10^{-2}/T$ $+7.684 \cdot 10^{-4}P$	32.15 $-3.388 \cdot 10^{-2}T$ $-1.379 \cdot 10^{-5}TP$ $+4.926 \cdot 10^{-11}TP^2$	n.a.	2.00 to 3.00	Cal.(water at several T, P[287])
diethyl ether	276	n.a.	1.01 or sat.	n.a.	2.17	n.a.	6.00 (293.16 K)	<5.00	n.a.

substance	ref	T/ K	P/ bar	$10^9 \cdot \mathbb{D}/(m^2 \cdot s^{-1})$	$E_{\mathfrak{D}}/$ (kcal·mol^{-1})	$V_{\mathfrak{D}}/$ (cm^3·mol^{-1})	$10^9 \cdot \mathfrak{D}_{11}/(m^2 \cdot s^{-1})$	% error	gradient evaluation
dioxane	334	n.a.	1.01 or sat.	n.a.	4.20	n.a.	1.00 (298.16 K)	n.a.	shape
	316	n.a.	1.01 or sat.	277.88	3.23	n.a.	n.a.	n.a.	shape (1.0578)
acetone	331,334	n.a.	<709.23	150	2.03	13.0	4.77 (298.16 K)	5.00 to 10.00	Cal.(water[339])? shape?
	316	n.a.	1.01 or sat.	379.80	2.64	n.a.	n.a.	n.a.	shape (1.0578)
	324	180 to 300	1.01	121 ± 10	2.00 ± 0.10	n.a.	n.a.	n.a.	shape (0.9699)
	276[b]	223.16 to 353.16	Sat	n.a.	2.38	n.a.	4.30 (293.16 K)	<5.00	n.a.
benzophenone	276[b]	297.16 to 399.66	1.01	n.a.	8.50 (298.16 K) 5.80 (373.16 K)	n.a.	0.455 (343.16 K)	<5.00	n.a.
cyclohexanone	543	260 to 440	Sat	660 ± 110	4.12 ± 0.2	n.a.	n.a.	n.a.	shape (0.9699)
α-picoline	316	n.a.	1.01 or sat.	275	3.00	n.a.	n.a.	n.a.	shape (1.0578)
pyridazine	334	n.a.	1.01 or sat.	n.a.	4.1	n.a.	0.83 (298.16 K)	n.a.	shape
pyrazine	334	n.a.	1.01 or sat.	n.a.	6.5	n.a.	5.30 (373.16 K)	n.a.	shape
acetonitrile	276	n.a.	1.01 or sat.	n.a.	2.45	n.a.	4.85 (303.16 K)	<5.00	n.a.
nitromethane	331	n.a.	0 to 506.63	1300	3.81	13.6 (0 bar) 16.0 (506.63 bar)	2.11 (298.16 K)	5.00 to 10.00	Cal.(water[339])? shape?
	324	220 to 370	1.01	160 ± 15	2.53 ± 0.15	n.a.	n.a.	n.a.	shape (0.9699)
nitrobenzene	324	270 to 435	1.01	670 ± 70	4.05 ± 0.15	n.a.	n.a.	n.a.	shape (0.9699)
tetramethyl tin	304[d]	247.30 to 373.80	1.00 to 2000	55.53	1.894 $-1.567 \cdot 10^{-1}/T$ $+1.087 \cdot 10^{-4}P$	4.547 $+4.905 \cdot 10^{-2}T$ $-2.48 \cdot 10^{-5}TP$ $+2.649 \cdot 10^{-12}TP^2$	n.a.	2.00 to 3.00	Cal.(water at several T, P[287])
chloroform	276	n.a.	1.01 or sat.	n.a.	2.54	n.a.	3.16 (303.16 K)	<5.00	n.a.
carbon tetrachloride	426	280.00 to 330.00	1.01	245.49	3.11	n.a.	n.a.	n.a.	shape (0.9221)
	23	290.00 to 350.00	1.01	246.72	3.11	n.a.	n.a.	n.a.	shape (0.8986)
dichloroethane (*sic*)	276	n.a.	1.01 or sat.	n.a.	2.90	n.a.	2.01 (303.16 K)	<5.00	n.a.
chlorobenzene	324[e]	220 to 400	1.01	360 ± 30	3.12 ± 0.15	n.a.	n.a.	n.a.	shape (0.9699)
	276[b]	298.16 to 373.16	1.01	n.a.	2.79	n.a.	2.35 (313.16 K)	<5.00	n.a.
deuterium	544	19.00 to 21.00	1.01	48	0.10	n.a.	n.a.	n.a.	n.a.
water	331,334	273.16 to 373.16	<709.23	n.a.	5.00 (273.16 K) 3.00 (373.16 K)	0.0	2.10 (298.16 K)	5.00 to 10.00	Cal.(water at 298.16 K[339])
	316	n.a.	1.01 or sat.	5730	4.60	n.a.	n.a.	n.a.	shape (1.0578)
	276[b]	273.16 to 403.16	Sat.	n.a.	5.15 (273.16 K) 3.62 (373.16 K)	n.a.	2.00 (293.16 K)	7.00	n.a.
hydrogen fluoride	441[f]	190 to 300 [322]	Sat.	740 ± 120	2.68 ±0.04	n.a.	n.a.	n.a.	shape (0.9699?[324])
metanol	276	n.a.	1.01 or sat.	n.a	3.18 (293.16 K) 3.46 (353.16 K)	n.a.	2.01 (293.16 K)	<5.00	n.a.
methanol-*d*	324	180 to 340	1.01	560 ± 30	3.21±0.10	n.a.	n.a.	n.a.	shape (0.9699)
etanol	276	n.a.	1.01 or sat.	n.a.	4.28 (293.16 K)	n.a.	0.98 (293.16 K)	<5.00	n.a.

substance	ref	T/ K	P/ bar	$10^9 \cdot \mathbb{D}/(m^2 \cdot s^{-1})$	$E_{\mathfrak{D}}/$ (kcal·mol^{-1})	$V_{\mathfrak{D}}/$ (cm^3·mol^{-1})	$10^9 \cdot \mathfrak{D}_{11}/(m^2 \cdot s^{-1})$	% error	gradient evaluation
					4.90 (363.16 K)				
n-propanol	276	n.a.	1.01 or sat.	n.a.	5.05	n.a.	0.48 (293.16 K)	<5.00	n.a.
n-butanol	276	n.a.	1.01 or sat.	n.a.	5.41	n.a.	0.35 (293.16 K)	<5.00	n.a.
cyclohexanol	543	350 to 440	Sat.	35000 ± 19000	7.8 ± 0.6	n.a.	n.a.	n.a.	shape (0.9699)
phenol	276[b, g]	313.16 to 401.16	1.01	n.a.	9.53 (293.16 K)	n.a.	0.78 (343.16 K)	<5.00	n.a.
					6.10 (373.16 K)				
phenyl salicylate	276[b]	293.16 to 373.16	1.01 or sat.	n.a.	11.10 (298.16 K)	n.a.	0.254 (333.16 K)	<5.00	n.a.
					5.65 (373.16 K)				
aniline	276[b, g]	297.16 to 400.16	1.01	n.a.	7.25 (293.16 K)	n.a.	1.32 (343.16 K)	<5.00	n.a.
					4.60 (373.16 K)				
acetic acid	276	n.a.	1.01 or sat.	n.a.	3.30	n.a.	0.99 (293.16 K)	<5.00	n.a.

[a] The activation volume of ref 542 is a correction of ref 320, so it is expected that the equation will be valid in the same temperature range. [b]Also in graphical form. See the text. [c] The integrated expression for mesitylene is $\mathfrak{D}_{11}=10^{-9}\exp(4.994-1343.33/T+2.643/T^2-0.3867P/T+407.6\cdot10^{-6}P+8.2944\cdot10^{-8}P^2-198.4\cdot10^{-15}P^3)$. [d] The integrated expression for tetramethyl tin is $\mathfrak{D}_{11}=10^{-9}\exp(4.017-953.37/T+39.444/T^2-0.0547P/T-590\cdot10^{-6}P+14.916\cdot10^{-8}P^2-10.624\cdot10^{-15}P^3)$. [e] This formula corrects the numerical values published previously by O'Reilly in ref 322. [f] These measurements were considered by O'Reilly better than those given graphically in ref 322. [g] Activation energies for diffusion were only provided at 373.16 K. Since the paper apparently demonstrated the applicability of the Stokes-Einstein equation to self-diffusion, we have taken the values at 293.16 K as the energies of the ratio between the viscosity and the absolute temperature, which were reported by the author.

2.3. Neutron scattering. When an atomic nucleus of a substance scatters an incident beam of neutrons, there is a response $S(\vec{Q},\omega)$which is a function of the momentum $\hbar\vec{Q}$ and the energy $\hbar\omega$ absorbed from or imparted to the neutrons[545,546]

$$S(\vec{Q},\omega) = \left\{\frac{b_{incoh}^2}{b_{total}^2} S_{incoh}(\vec{Q},\omega) + \frac{b_{coh}^2}{b_{total}^2} S_{coh}(\vec{Q},\omega)\right\} \quad (8)$$

$$\vec{Q} = \overrightarrow{k_i} - \overrightarrow{k_s} \quad (9)$$

$$\omega = \frac{\hbar}{2m_n}\left(\left|\overrightarrow{k_i}\right|^2 - \left|\overrightarrow{k_s}\right|^2\right) \quad (10)$$

where $\hbar$ is the rationalized Planck's constant, m_n the neutron mass, $\overrightarrow{k_i}$ and $\overrightarrow{k_s}$ the wave vector of the incoming and scattered neutrons, respectively (being $\left|\overrightarrow{k_i}\right|$ and $\left|\overrightarrow{k_s}\right|$ their modules) and b the scattering length of the atom. The subscripts "coherent" and "incoherent" refer to the type of scattering,[547] which is coherent if the neutrons are scattered individually by each atom (providing information of their individual motion, i.e., self-diffusion, rotation, vibration, jumps, spin changes, etc.) and is incoherent if there is interference between the scattered waves of the different atoms (showing their collective motion or spatial distribution).

Vanadium and hydrogen are the only naturally occurring elements for which the scattering is predominantly incoherent ($b_{incoh}>>b_{coh}$), but fortunately, the large incoherent scattering length of the protons makes the coherent contribution almost negligible from other nuclei in molecules that contain hydrogen[545] and the scattering spectra will mainly reflect the motions of the individual hydrogen atoms[548-550]

Additionally, the incoherent part can be expressed in terms of the intermediate scattering function $I_s(\vec{Q},t)$ as

$$S_{incoh}(\vec{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I_s(\vec{Q},\omega) exp\,(-i\omega t)dt \quad (11)$$

where translational, rotational, vibrational and all the individual motions are represented. As a working hypothesis, it is commonly supposed that these motions are dynamically independent (or uncoupled) so that the total I_s can be factorized as the product of separate functions

$$I_s(\vec{Q},\omega) = I_s^{trans}(\vec{Q},\omega)\cdot I_s^{rot}(\vec{Q},\omega)\cdot I_s^{vibr}(\vec{Q},\omega)\cdots \quad (12)$$

The main disadvantage of the neutron scattering is that theoretical models have to be assumed for these functions, where not only $\mathfrak{D}_{11}$ is present, but also a rotational diffusion, characteristics distances, relaxation times and other model-dependent parameters. Moreover, corrections must be made for instrumental resolution, the scattering due to the sample container, multiple scattering and self-shielding[546]

The quasielastic part of the spectrum is the peak generated mainly by the translational contribution, and is prominent at low values of the momentum module, $|\vec{Q}|$. In the ideal case, the effects of vibrations and rotations are fully negligible, and $I_s = I_s^{trans}$. If the atom suffers random alterations of velocity in brief collisions occurring at random times (i.e. obeys Fick's Law), then

$$I_s^{trans}(\vec{Q},\omega) = \exp\left(-\mathfrak{D}_{11}|\vec{Q}|^2 t\right) \tag{13}$$

and the resulting profile is a simple Lorentzian

$$S_{incoh}(\vec{Q},\omega) = \frac{1}{\pi}\frac{\mathfrak{D}_{11}|\vec{Q}|^2}{\omega^2 + \left(\mathfrak{D}_{11}|\vec{Q}|^2\right)^2} \tag{14}$$

whose width at half-maximum ($\omega_{1/2}$) verifies that

$$\omega_{1/2} = 2\mathfrak{D}_{11}|\vec{Q}|^2 \tag{15}$$

This was the procedure followed by Chen et al.[551] to determine the self-diffusion of supercritical hydrogen at (78 and 293) K and pressures from (13.2 to 197.2) MPa with an accuracy of 10%.

Other researchers, who assumed that eq 15 was valid for liquids (at least, when $|\vec{Q}|^2 \rightarrow 0$) and also neglected the non-translational contributions or empirically removed them as background, found $\mathfrak{D}_{11}$ values close to those derived from tracer methods or nuclear magnetic resonance in the cases of cyclopropane,[358] cyclopentene,[483] water,[552,553] and methanol,[554] but observed a considerable disagreement for other compounds, such as pentane,[548] cyclopentane,[550] cyclohexane,[550] toluene,[555] ethanol,[554] pentanol,[554] and glycerol.[548] The reason is that the simple diffusion model is not always obeyed,[556-559] nor even at low values of the momentum module, and that other substance-dependent parameters have to be included in eq 15. Since these parameters change with temperature, and it is not possible to known a priori the applicability of the models and/or simplifications,[560-562] the neutron scattering cannot be considered properly a measurement technique, except at certain conditions (e.g., those of Chen and co-workers for hydrogen).

In fact, neutron scattering is a technique that needs the self-diffusion coefficients to validate theories and approximations. The normal procedure when dealing with it is to assign mathematical expressions to all parts of eq 12 and to the coherent contribution, if necessary, and then (i) to obtain $\mathfrak{D}_{11}$ and other fitting parameters from the experimental spectrum and to compare the calculated self-diffusion coefficients with those available in the literature,[547,562-568] or (ii) to take diffusivities from the literature, to solve eq 8 and to compare the calculated $S(\vec{Q},\omega)$ with the experimental one.[569-574] Therefore, in the Supporting Information, we have only included the aforementioned hydrogen of Chen et al.[551]

3. GENERAL CONSIDERATIONS

In this section, we will make a brief overwiew of the compiled self-diffusivities. It will be mainly focused on general trends and on detecting the strongest discrepancies between the different sources for the same substance. A detailed analysis to determine which experimental points are closer to the real diffusivities is beyond the scope of this study, since not only the data from several researchers can display considerable differences, but also those measured by the same authors in different papers (see, for example the alkanes of von Meerwall,[469,471,473] the alkanes of Emel'yanov,[465,468] the acetone of Le Bihan,[246,389,390] the tri-*n*-butyl phosphate of Pronin and Vashman,[348,401] and the 1-octanol and the fatty acids of Iwahashi;[29,347,450,457,458,533,534,541] they, unlike others such as Wang,[191,192,195,198] Hayamizu,[24,387,459,460] Anderson,[518-520] Zykov,[417,461] Yoshida,[372,432] or O'Reilly,[322,441] did not specifically say that some of their measurements were incorrect or inaccurate)

For this comparison, some densities or temperatures of methane, ethylene, saturated xenon, saturated argon, carbon dioxide, and hydrogen which were not provided by the articles themselves are necessary. They were taken from the works of Setzman and Wagner,[575] Smukala et al.,[576] Sifner and Klomfar,[577] Tegeler et al.,[578] Span and Wagner,[579] and Leachman et al.,[580] respectively, changing the critical constants if necessary. These densities or temperatures have been listed in the Supporting Information colored in red. Additionally, $^{13}CO_2$ has been treated as CO_2 because the similarity of their critical properties and the small mass difference (only of 2.2%).[27]

3.1. Water. As referred to in section 2.2, Weingärtner[285] compared the tracer and spin-echo diffusivities of water available until 1982 and concluded that the extrapolated values of Mills[40] were the best ones. Previous studies, focused on atmospheric pressure and room temperature[425] or on the pressure dependence at 298 K[202] had disregarded the points of Wang,[198] Wang et al.,[195] Simpson and Carr,[339] Trappeniers et al.,[326] Benedek and Purcell,[504] Cuddeback et al.,[194] Kisel'nik et al.,[526] and McCall et al.[331] Subsequent works, such as those of Harris and Newitt[430] and Yoshida et al.[372] confirmed the good agreement between their measurements and the data of Angell et al.,[527] Harris and Woolf,[287] Hausser et al.,[269] Prielmeier et al.,[293] and Krynicki et al.,[286] although the pressurized diffusivities of Krynicki below 298.16 K are erroneous. The temperature dependence of $\mathfrak{D}_{11}$ at 101.325 kPa is also correct for Ertl and Dullien,[378] Becker et al.,[249] Holz et al.,[307] Tofts et al.,[315] and Hardy et al.[529]

Therefore, in those papers of the following sections that calibrated the coils with the water of Simpson and Carr ($2.13\cdot10^{-9}$ $m^2\cdot s^{-1}$ at 298.16 K) or of Trappeniers et al. ($2.51\cdot10^{-9}$ $m^2\cdot s^{-1}$ at 298.16 K), we have divided the corresponding $\mathfrak{D}_{11}$ values by 0.9265 or 1.0918, respectively, in order to obtain self-diffusion coefficients as if the apparatuses had been calibrated with the water of Mills ($2.299\cdot10^{-9}$ $m^2\cdot s^{-1}$ at 298.16 K). These corrections have not been included in the Supporting Information, and have not been applied to those studies which

evaluated *G* by the shape of the echo-spin either, since in this case, the presence of systematic error is not always assured (see Section 2.2).

With regards to heavy water, it has to be said that, within the experimental uncertainties, all the liquid diffusivities at atmospheric/saturation pressure are in relatively good agreement, except those of Wilbur et al.[435] around (363.16 to 393.16) K (the uncorrected ones of Yoshida et al.[432] have not been taken into account). At high pressures, the concordance gets worse, especially between Prielmeier-Arnold[293,438] and DeFries and Jonas[436] in the range (258.16 to 278.16) K and between Wilbur et al.[435] and Prielmeier et al.[293] at (363.16 to 423.16) K.

3.2. Other saturated liquids. For these comparisons, extrapolation of some high-pressure diffusivities to low pressure has been carried out.[35,108,412,413]

At first glance, all the coefficients of Kitchlew and Nageswara Rao[484] are systematically higher than those determined by other authors for the same substances (assuming that the equations of Samigullin for *m*-xylene and *p*-xylene are valid in the same temperature ranges). The values obtained for hexane by Vashman and Pronin,[348] for dodecane by Emel'yanov et al.,[468] for tetratriacontane by Yamakawa et al.,[354] for dioxane by Clemett,[491] for dimethylsulfoxide by Merbolt et al.,[247] for tri-*n*-butyl phosphate by Pronin and Vashman,[401] for fluoroform by Chaffin and Hubbard,[403] for *tert*-butyl chloride by Grochulski et al.,[496] for xenon by Yen and Norberg,[420] for carbon dioxide by Krynicki,[512] for methanol by Sandhu,[501] and for ethanol, propanol and butanol by Powles and Cutler[443] are very high when also compared with the measurements from other researchers. On the other hand, the methane of Gaven et al.,[226] the decane of Emel'yanov et al.,[468] the toluene of Reimschüssel and Hawlicka,[217] the acetone determined by TDPFG-Im[245] and SS-MRE,[236] and the xenon of Streever and Carr[410] are considerable lower than the rest.

It can also be observed that for hexane, octane, decane, tetradecane, tetracosane, neopentane, isopentane, 2,2-dimethylbutane, nitromethane, *N*,*N*-dimethylformamide, dimethylsulfoxide, dichloromethane, chloroform, *tert*-butyl chloride, hexafluorobenzene, chlorobenzene, octanol, stearic acid, oleic acid, and eleaidic acid, there was good concordance between the several sources at low temperatures, but at higher ones, some sets of diffusivities display higher activation energy than the others. See, for example, Figure 1. Near the critical temperature, the cyclohexane, benzene and toluene of Panchenkov et al.[365] are (20 to 30) % higher than those of Yoshida et al.,[372] Hausser et al.,[269] Asahi et al.,[267] and Shimokawa,[486] although at lower temperatures, the data of Yoshida, Hausser and Asahi are 10% above the values of Panchenkov. These discrepancies are frequently attributed to convection (especially when nuclear magnetic resonance is utilized) which causes measured diffusivities to be above the real ones,[351,364,489,581,582] but this fact does not guarantee that the lower values are always the correct ones: some investigators who perceived that their points were higher than those expected did not detect convection in their devices[420,268] and other experimental errors can decrease the experimental results below the true self-diffusion coefficients.[125,372,432]

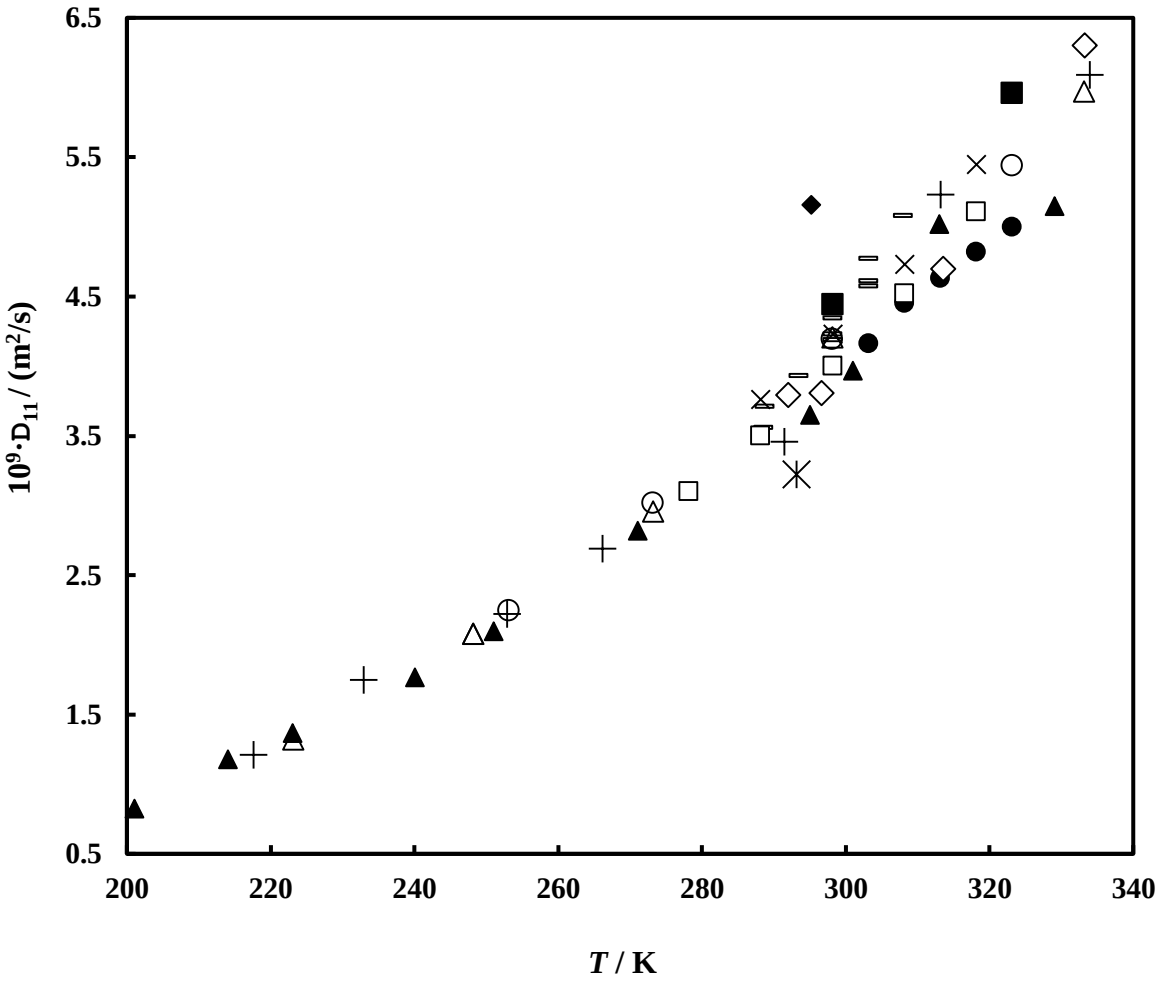

Figure 1. Self-diffusion of hexane at saturation/atmospheric pressure as a function of the temperature: open rectangle, Hawlicka and Reimschüssel;[113] ▲, Bachl;[256] ○, Brüsewitz and Weiss;[301,302] ●, Kasahara et al.;[310] +, Douglass and McCall;[328] ■, Iwahashi et al.;[347] ◆, Vashman and Pronin;[348] △, Harris;[349] ×, Marbach and Hertz;[350] ∗, Agishev and Emel'yanov;[465] ◇, Panchenkov et al.;[467] □, Emel'yanov et al.[468]

For cyclohexanone, tetramethyl lead, bromoform, iodomethane, and krypton the differences among the few available diffusivities is so strong, that it is not possible to estimate $\mathfrak{D}_{11}$ with less than 20% error even at a single temperature.

Based on the experimental arrangements, Mills[425] concluded that, at 298.16 K, the argon of Cini Castagnoli[154] was more accurate than that of Corbett and Wang[153] and of Naghizadeh and Rice.[35] By comparing calculated activation energies, Freer and Sherwood[125] stated that the cyclohexane data of McCall et al.,[331] Hawlicka and Reimschüssel,[113] and Anderson and Gerritz[274] were less reliable than those of others, and said the same for the benzene of Graupner and Winter,[126] Hiraoka et al.,[128] and McCall et al.[331]

3.3. Compressed liquids. Ethane of Wade and Waugh,[463] benzene of Hiraoka et al.[128] and McCall et al.,[331] carbon tetrachloride of Watts et al.,[145] carbon disulfide of Koeller and

Drickamer,[181] and methanol of Hiraoka et al.[212] have been critizised and considered erroneous by Greiner-Schmid et al.,[288] McCool et al., [133] McCool and Woolf,[148] Woolf,[72] and Hurle et al.,[583] respectively. The concordance among the rest of sources for each liquid is relatively good, except for the alkanes of McCall and coworkers,[320,328,331,542] the methanol-*d* of Jonas and Akai above 283 K,[446] the 2,2-dimethylbutane, and the cyclohexane. In the first case, the agreement with the paraffins of Harris,[137,349] Bachl,[256] Arkhipov et al.,[346] Marbach and Hertz,[350] and Brüsewitz and Weiss[302] is only good at certain temperatures, and for the isopentane of Enninghorst[356] there is no agreement at all. In the case of methanol-*d*, the high-temperature points of Jonas and Akai are (12 to 25) % higher than those of Hurle et al.[213] and of Karger et al.[295] For 2,2-dimethylbutane and cyclohexane, each author obtained a different trend, as shown in Figures 2 and 3, respectively.

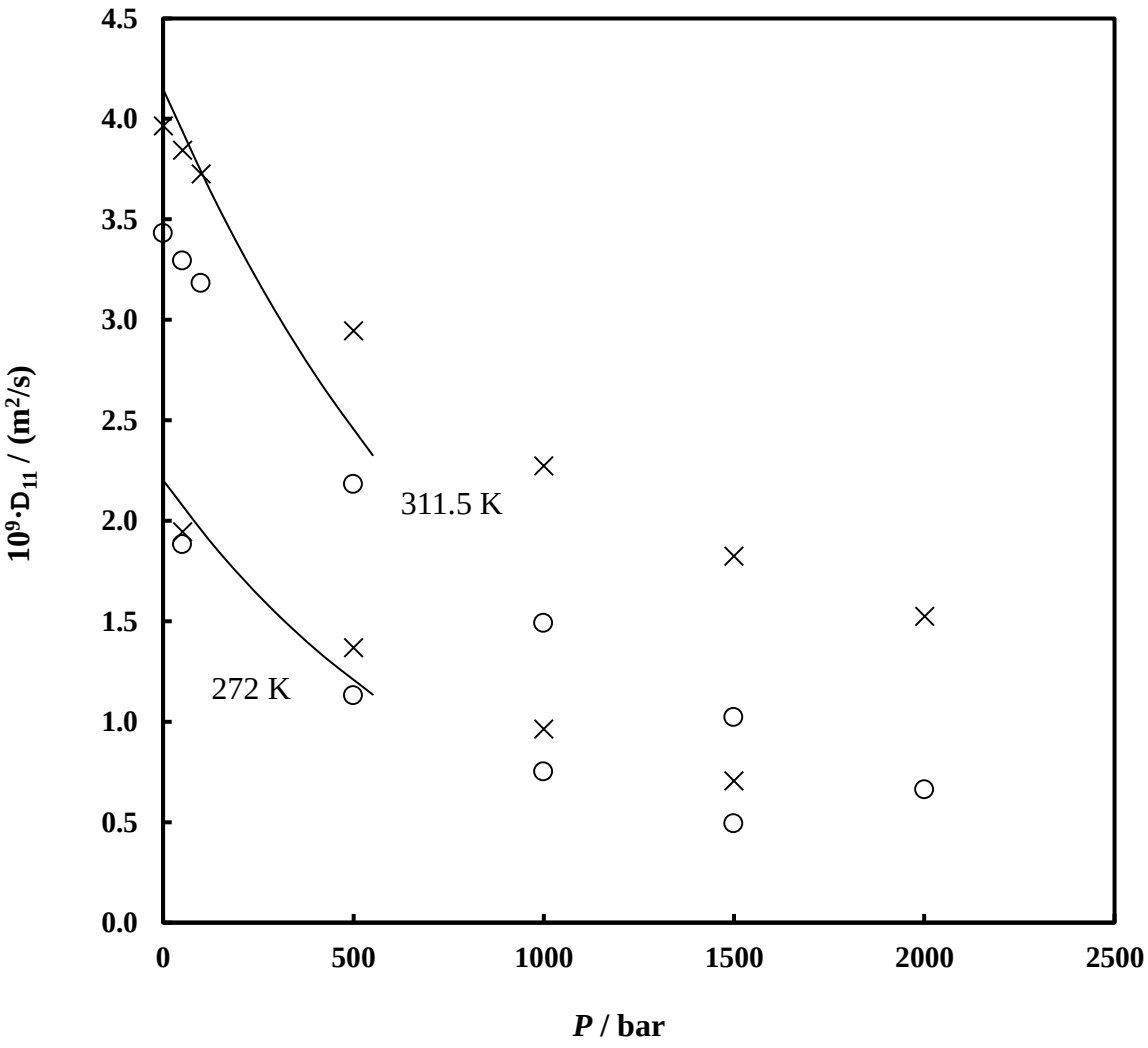

Figure 2. Temperature and pressured dependence of self-diffusion of 2,2-dimethyl butane according to three sources: ○, Bachl;[256] ×, Polzin and Weiss;[304] solid line, McCall et al.[320] For the sake of comparison, some points have been interpolated.

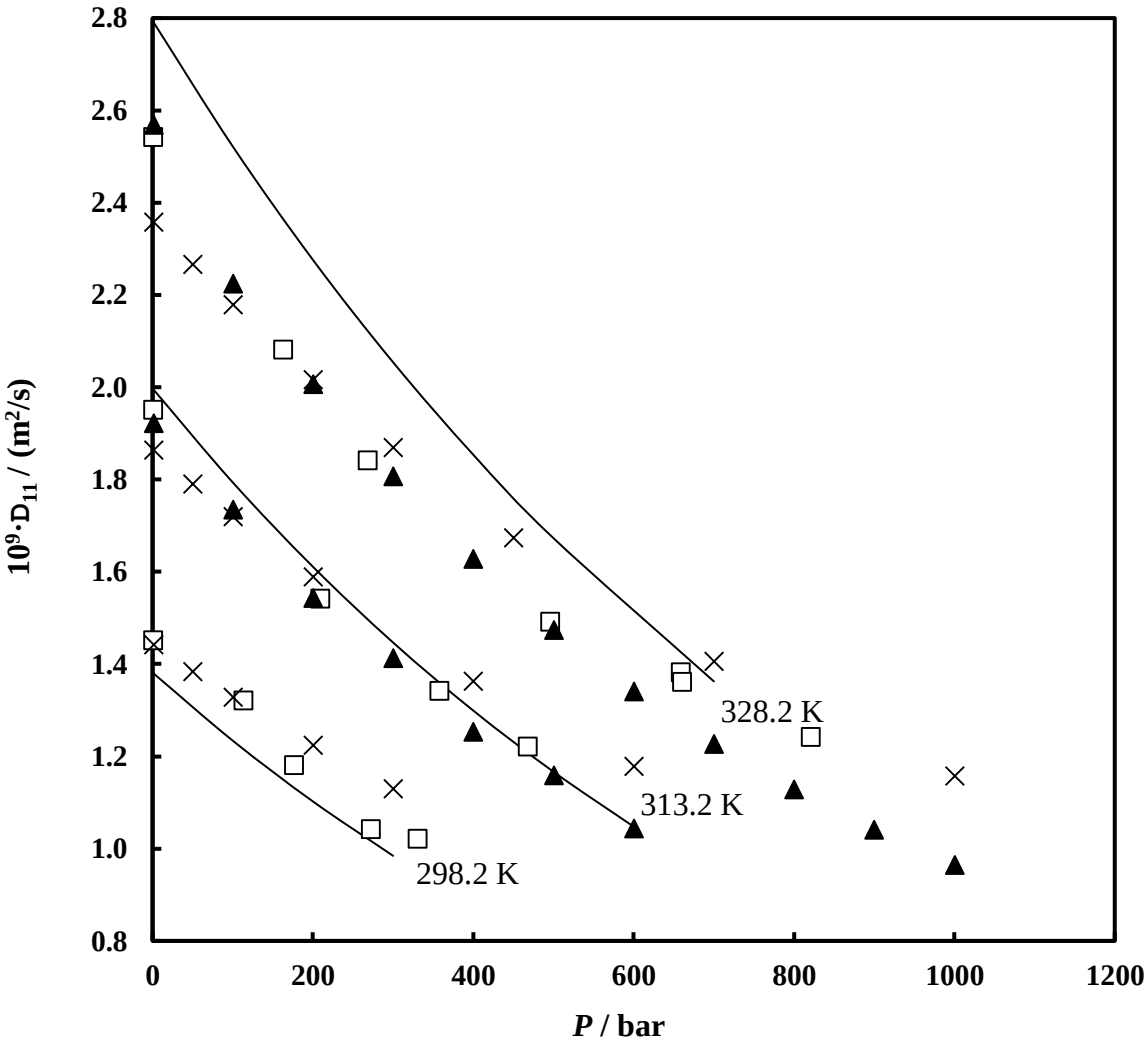

Figure 3. Temperature and pressure dependence of the self-diffusion of cyclohexane according to four sources: □, McCool and Woolf;[124] ×, Polzin and Weiss;[304] solid line, McCall et al.;[331] ▲, Jonas et al.[367] For the sake of comparison, some points have been interpolated.

On the other hand, and within an experimental error of 10%, there is no difference between the self-diffusivity of normal hydrogen and a mixture with other proportions of *ortho*- and *para*-hydrogen at constant temperature and density.[515]

3.4. Vapors and gases at low density. For each substance, all the points from the different sources are in relatively good agreement (5 to 10%), except the value of Hutchinson

for argon at 90.16 K[67] and the xenon of Benenson et al.[163] and of Groth and Harteck.[41] Nonetheles, Hutchinson and Benenson themselves doubt the reliability of these measurements.

Mueller and Cahill[76] questioned their acetylene also because experimental problems. Unfortunately, no more data from other investigators are available in the same conditions to confirm or deny their suspicions.

Additionally, it has to be pointed out that the high-temperature data of Ember et al.[175] and Pakurar and Ferron[177] were cast in doubt by Bock et al.,[584] who were able to reproduce the low-density viscosity of carbon dioxide within a 1% error for (1000 to 1500) K by calculations with the intermolecular potential of Bukowski, but obtained deviations of (13 to 43) % for the self-diffusivities of the aforementioned researchers.

The applicability of eq 2 to the hydrogen isotopes has been discussed by Amdur and Beatty,[81] Mason et al.[36,82] and Reichenbacher et al.[187] The first two groups observed differences of (4 to 6) % and stated that not only the mass, but also the characteristic energies and molecular diameters changed considerably; whereas the last group affirmed that, although eq 2 was not strictly valid, the deviations were around 2% and attributed the results of Amdur and Mason to experimental errors.

As in the case of the compressed liquid, $\rho\mathfrak{D}_{11}$ for hydrogen is independent of the concentration of the ortho species at a given temperature.[515]

3.5. Compressed gases and vapors. Previous studies[27,585] have rejected the methane of Cini Castagnoli et al.[216] and the carbon dioxide of Duffield and Harris[89] since these authors were the only ones to see an anomaly of the self-diffusion (similar to that of viscosity and thermal conductivity) in the vicinity of the critical point. Other researchers[412,586] have considered erroneous the methane and carbon dioxide of Drickamer and coworkers[86,104,173,174] as well, but because their points were 50% lower than the rest of the references.

In order to afford a better comparison among the literature, we have plotted $\rho\mathfrak{D}_{11}$ vs ρ for some substances, as in Figure 4. At first glance, it is clear that the ethylene and sulfur hexafluoride of Hamann[476,477] and the carbon dioxide of Krynicki et al.[512] are 20-40% higher than those from other sources, although if the values of Hamman are divided by 1.1091 (see Table 5), the ethylene becomes closer to the data of Takahashi,[118] Arends,[357] and Peereboom.[479] This improvement can be also appreciated in Figure 4, where the data of Oosting and Trappeniers[257] around 298 K, divided by 1.0918, approach the more recent values of Harris[342] and Greinerd-Schmidt.[288] Nonetheless, the quality of the correction is not constant, since at low temperatures, the concordance between Harris[343] and Oosting[257] is good without taking into account this factor.

On the other hand, it is curious that at 298 K, all the diffusivities obtained by nuclear magnetic resonance tend to a low-density value below that of Winn,[65] which is in accordance with the extrapolation of Takahashi[107] and the measurements in methane-d_4 of Mueller[76] and Vugts.[45] However, this cannot be due to differences between the tracer motion and the spin echo, since the tracer chromatographic method of Hu and Kobayashi[106] provides the same result as the nuclear magnetic resonance, and at lower temperatures, the agreement among the several

data sets is better, all them merging into the single point of Winn around 194 K. We have seen the same discrepancies regarding the low-density limit for the carbon dioxide of Etesse et al.[412] and for the hydrogen of Chen et al.[419] as well, but not for ethylene or xenon.

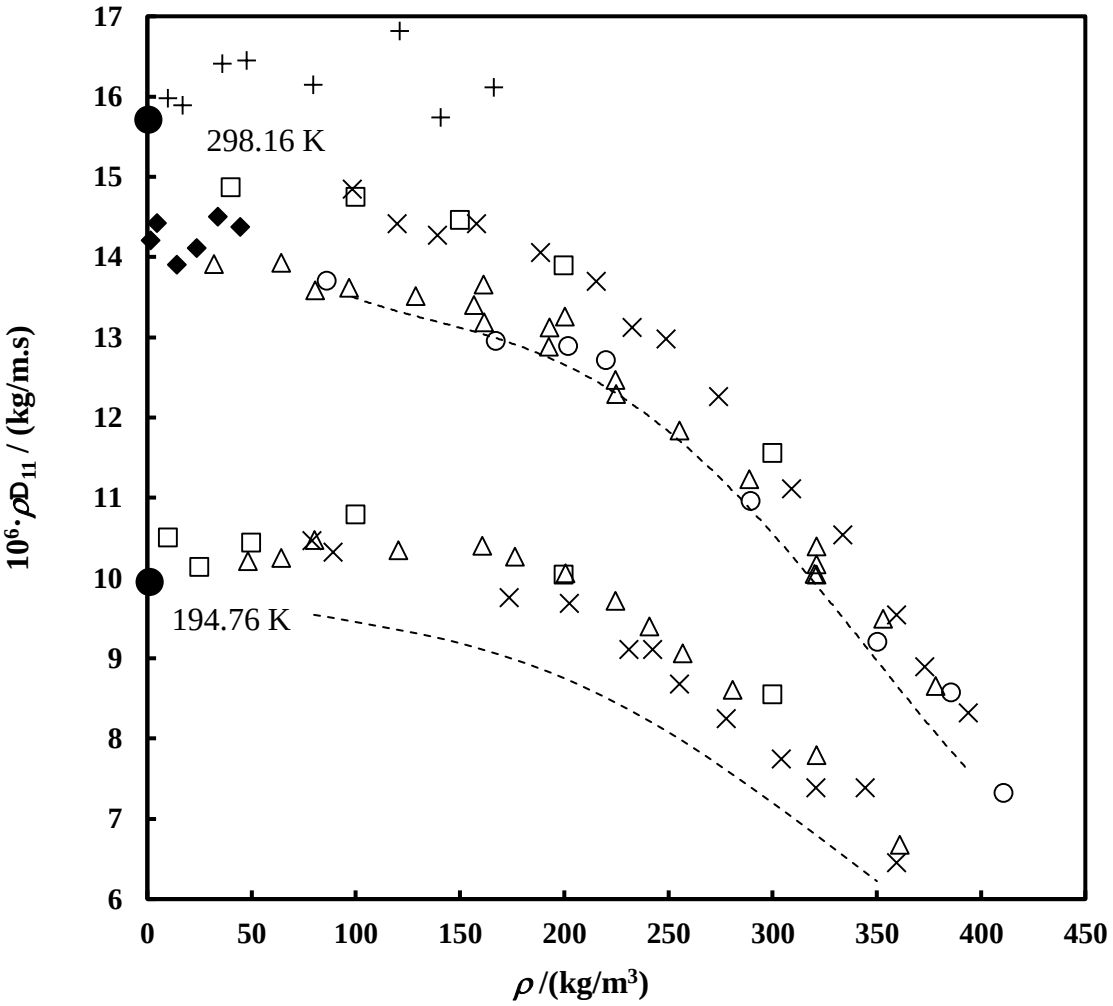

Figure 4. Density dependence of the group $\rho\mathfrak{D}_{11}$ for methane according to several sources: ●, Winn;[65] ◆, Hu and Kobayashi;[106] +, Takahashi;[107] □, Dawson et al.;[283] ×, Oosting and Trappeniers;[257] ○, Greiner-Schmid et al.;[288] △, Harris.[342,343] For the sake of comparison, some points have been interpolated. The dotted line corresponds to the data of Oosting and Trappeniers divided by the factor 1.0918.

In the case of carbon tetrafluoride, where only two sets of supercritical points are available, it is not possible to know which are correct, since those of Khoury and Kobayashi[284] are systematically (20 to 40) % lower than those of Has and Lüdemann.[291] For hydrogen, the neutron scattering[551] produced results (5 to 10) % higher than the spin-echo technique,[419] the former being in better agreement with the low-density tracer diffusivities than the latter.

4. CONCLUSIONS

Self-diffusion in fluids has been reviewed. The most widely studied substance is water, followed by benzene and cyclohexane. The preferred measurement technique is the spin-echo, in the pulsed field gradient version of Stejskal-Tanner or in one of its numerous improvements, since it does not need the introduction of a new species in the system (tracer methods) nor the assumption of complex mathematical models for the molecular motions (neutron scattering). Additionally, we hope that the thousands of experimental data compiled as Supporting Information will facilitate the understanding of this fundamental transport property for future researchers.

ASSOCIATED CONTENT

Supporting information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jced.5b00323.

Properties of the considered substances and all the data of Tables 1,2,4, and 5, together with the points obtained by Chen et al.551 for hydrogen through neutrón scattering (ZIP)

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Notes

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TABLE OF CONTENTS GRAPHIC

SELF-DIFFUSION IN MOLECULAR FLUIDS AND NOBLE GASES: AVAILABLE DATA

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