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Donald R. Burgess Jr.

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Donald R. Burgess Jr.
Chemical Sciences Division
Material Measurement Laboratory

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Author ORCID iD
Donald R. Burgess Jr.: 0000-0002-3428-6540

Abstract

In this work, we compiled and evaluated both self-diffusion and binary-diffusion coefficients *D* for gases as a function of temperature. The tables in this paper have approximately 300 individual diffusion coefficients for a wide range of chemical classes: rare gases, small H/O/N/S species, hydrocarbons, and oxygen-, nitrogen-, and halogen-substituted hydrocarbons. The recommended values for the diffusion coefficients are for standard room temperature 298.15 K (D_{298}) and standard atmospheric pressure (101.325 kPa). We also provide expressions for many of the diffusion coefficients as a function of temperature, where available in the literature.

Keywords

Self-diffusion coefficients; binary-diffusion coefficients; temperature-dependent diffusion coefficients; gases; small molecules; hydrocarbons; substituted-hydrocarbons; critical evaluation.

Table of Contents

1. Introduction

In this work, we compiled and evaluated both self-diffusion and binary-diffusion coefficients D for gases as a function of temperature and provide recommended values for the diffusion coefficients at standard room temperature 298.15 K (D_{298}) and standard atmospheric pressure (101.325 kPa). We also provide recommended temperature-dependent expressions for many (about 30 %) of the diffusion coefficients. In the tables, the substances are ordered by chemical class (e.g., Rare Gases, Small Molecules, Halogen Species, NO_x species, Alkanes, Alkenes, Alcohols, Ethers, etc.) and then by molecular weight. The tables in this paper have approximately 300 individual diffusion coefficients.

Throughout this work, we used absolute temperatures T in K, not the Celsius temperature scale with t in °C. Where possible, the temperature dependencies of the diffusion coefficients were fit in three different ways. (1) $\ln(D) = A + B/\mathrm{T} + C\cdot\ln(T)$, an extended expression over the entire temperature range, (2) $D = A_n\cdot(T/298.15)^n$, a power-law expression over the entire temperature range, and (3) $\ln(D) = A + B/T$, a fit just near room temperature in order to calculate a precise value for the diffusion coefficient at room temperature (D_{298}) and to provide a measure of the activation barrier (E) to diffusion ($D = A\cdot e^{-E/RT}$).

We estimated the generic expanded uncertainty for the diffusion coefficients at T = 298.15 K to be up to about U/D_{298} = (15 to 20) % based on deviations from correlations. The individual uncertainties, however, are probably in the range of (5 to 10) %. This (15 to 20) % broad uncertainty estimate excludes the rare gases and small molecules such as H_2, N_2, O_2, NH_3, CH_4, ethane, ethylene, acetylene, CO, and CO_2, where it is much more difficult to assign uncertainties based on simple correlations.

2. Overview

2.1. Diffusion Coefficients

In the tables in this paper, for each substance, the bath gas is given in the column "Bath" – for self-diffusion coefficients, the bath gas is same as the substance. Note that to a very good approximation for a low-density binary gas, the diffusivity of A in B is the same as the diffusivity of B in A – the difference is generally much less than 1 %, which is significantly less than the uncertainties in the experimental diffusion coefficients which are on the low end about (2 to 5) % and can be up to (10 to 15) %.

For each substance, several different typical diffusion-coefficient expressions have been employed to fit the diffusion coefficients as a function of temperature. In this work, we used absolute temperatures T in K, not the Celsius temperature scale with t in °C.

(1) They were fit over the entire temperature range that was reported using the extended diffusion expression $\ln(D) = A + B/T + C\cdot\ln(T)$.
(2) They were fit over the entire temperature range using the power-law expression $D = A_n\cdot(T/298.15\ \mathrm{K})^n$.
(3) They were also fit just near room temperature using the simple form of the diffusion expression $\ln(D) = A + B/T$ in order to extract a precise value for the diffusion coefficient at 298.15 K (D_{298}). This is necessary because the slopes (B) of these curves increase substantially with temperature, for example, for a curve with a $T^{2.0}$ dependence, the activation energy (E) for diffusion $D = A\cdot e^{-E/RT}$ is about $E(\mathrm{kJ\ mol^{-1}}) = (T/60)$ or (5.0, 8.5, 16.5, and 24.9) kJ mol^{-1} at (300, 500, 1000, and 1500) K, respectively. In order to have a systematic way of providing D_{298}, we chose the temperature ranges of these fits to be over about a 100 K range from about 273 K to 373 K using the temperatures reported closest to those values. In cases where the lowest temperature reported was above 273 K, we fit from the lowest temperature reported to the closest temperature to 473 K. Here, we used the power-law expression $D = A_n\cdot(T/298.15\ \mathrm{K})^n$ to fit the diffusion coefficients and computed D_{298} from this fit, that is $D_{298} = A_n$.

In the tables, the diffusion coefficients from the fits are valid over the temperature range provided in the column T(K). For all mixtures, a diffusion coefficient (D_{ref}) is given at a reference temperature. For those mixtures with expressions for the diffusion coefficient, this reference temperature is T = 298.15 K, while for all others, the reference temperature is that given in the T(K) column.

2.2. Uncertainties in Diffusion Coefficients

We estimated the expanded uncertainty for the diffusion coefficients at T = 298.15 K to be up to about U/D_{298} = (15 to 20) %, based on deviations from various correlations that we tried – this estimated uncertainty was simply based on deviations from simple correlations (in order to screen for outliers). The individual uncertainties are more likely in the range of (5 to 10) %. Where experimental uncertainties are given in the original sources, we provide these

uncertainties. The (15 to 20) % broad uncertainty estimate excludes the rare gases and small molecules – such as H_2, N_2, O_2, NH_3, CH_4, ethane, ethylene, acetylene, CO, and CO_2, where it is more difficult to assign uncertainties based on simple correlations. Of the roughly 300 diffusion coefficients, approximately 45 of them have assigned uncertainties with the first two quartiles, the third quartile, and the fourth quartile having average uncertainties of 2 %, 4 %, and 10 %, respectively.

In the work of McGivern and coworkers, the expanded uncertainties (*U*) are about 6 %, (12 to 15) %, (3 to 4) %, and (5 to 8) % in Ref. 1, Ref. 2, Ref. 6, and Ref. 8, respectively. For the diffusion coefficients from the sources where the diffusion coefficients were calculated from first principles (Refs. 10-31), the inherent uncertainties are very small – much less than 1 %. However, we provide the uncertainties in the experimental determinations as estimated by the authors in Refs. 10-31 from the deviations of their predicted values and the experimental determinations.

2.3. Diffusion Coefficients Calculated from First Principles

In Refs 10-31, highly accurate diffusion coefficients were calculated from collision cross-sections derived using first principles using intermolecular potential energy surfaces (PES) and gas kinetic theory. This methodology can calculate thermodynamic and transport properties including the second virial coefficient *B*, shear viscosity η, thermal conductivity λ, and diffusion coefficients *D*.

The potential energy surfaces can be accurately calculated using quantum-chemical *ab initio*, semi-empirical, classical, or semi-classical methods. An important aspect of the derivation of diffusion coefficients is that the second virial coefficient *B* in the virial expansion provides a first-order correction to the ideal gas law (real versus ideal densities),

$$(P/\rho_m RT) = 1 + B(T)\rho_m + C(T)\rho_m^2 + \ldots$$

where *P* is pressure, ρ_m is molar density, *R* is the gas constant, *T* is temperature, and *C* is the third virial coefficient. *B* is a simple function of the collision partners.

Transport properties, such as diffusion coefficients, which have been derived from first principles agree with experimental measurements which generally have uncertainties on the order of (2 to 4) %. However, transport properties calculated from first principles are believed to be accurate to less than 1 % for atoms and small, nearly rigid molecules. Calculated diffusion coefficients are a function of temperature *T*, the reduced mass of the collision partners $\mu(m_a,m_b)$, the average molecular speed $\langle v_{ab} \rangle$ (from gas kinetic theory), the molar density (from the second virial coefficient *B*), and the collision cross-sections σ (from first principles using the PES).

2.4. Dependence of Diffusion Coefficients on Molecular Weight and Compound Class

We found that overall that the diffusion coefficients (D_{298}) for the alkanes in N_2 followed an approximate empirical relationship:

$$D_{298}(\text{alkanes}/N_2) = 1.45 \cdot M^{-0.656}\ \text{cm}^2\ \text{s}^{-1}$$

where M is the molecular weight of the substance in g mol^{-1}. Note that this correlation ignores the cross-section dependence of the diffusion coefficient, among other factors. This simple empirical relationship has the diffusion coefficients decreasing slightly more strongly with molecular weight than $D \sim M^{-1/2}$, which is a baseline dependence from gas kinetic theory. In contrast, the observed diffusion coefficients in He for the alkanes are about a factor of 3.33±0.2 times larger than in N_2 (see Figure 1 for $D_{298}(M)$ in He and N_2):

$$D_{298}(\text{alkanes}/\text{He}) = 4.26 \cdot M^{-0.625}\ \text{cm}^2\ \text{s}^{-1}$$

This ratio is consistent with the scaling of diffusion coefficients with the reduced mass of the substance and bath gas, M_1 and M_2, respectively, and the average kinetic collision diameter d_{12}:

$$D \sim (1/d_{12})^2\,(1/M_1 + 1/M_2)^{1/2}$$

Utilizing collision diameters for He, N_2, propane, and heptane of 2.60 Å , 3.67 Å, 4.84 Å, and 5.72 Å (and interpolating/extrapolating for the other alkanes),[38] we found the ratios of D_{298} in He versus N_2 to be 2.83, 2.92, and 2.98 for propane, *n*-butane, and *n*-pentane – or close to the 3.33 ratio found experimentally. For the mass dependence of D_{298} for the alkanes in He and N_2 scaled by the collision cross-section, we found:

$$(\pi d_{12})^2 \cdot D_{298}(\text{alkanes}/\text{He}) \approx 76.6 \cdot M^{-0.393}\ \text{cm}^2\ \text{s}^{-1}\ \text{Å}^2$$

and

$$(\pi d_{12})^2 \cdot D_{298}(\text{alkanes}/N_2) \approx 38.0 \cdot M^{-0.452}\ \text{cm}^2\ \text{s}^{-1}\ \text{Å}^2$$

with the dependence of the mass (M) of the substance decreasing slightly less strongly than $D \sim M^{-1/2}$. In short, we believe that the experimental diffusion coefficients for the alkanes are consistent with the masses and kinetic collision cross-sections of the substance and bath gas.

We also considered the molecular weight dependence of D_{298} on chemical compound class and find that as the compounds become more polar that there is a slightly stronger dependence of the diffusion coefficients on molecular weight (M).

$$D_{298}(\text{Class}) = a \cdot M^b \text{ cm}^2\text{s}^{-1}$$

Mass Dependence of D_{298} by Compound Class

Compound Class	Bath	*a*	*b*
Alkanes	Air	1.35	-0.656
Alkenes	Air	1.84	-0.702
Subst-Benzenes	Air	4.18	-0.869
Esters	Air	4.85	-0.899
Alcohols	Air	4.36	-0.916
Alkanoic Acids	Air	8.73	-1.050

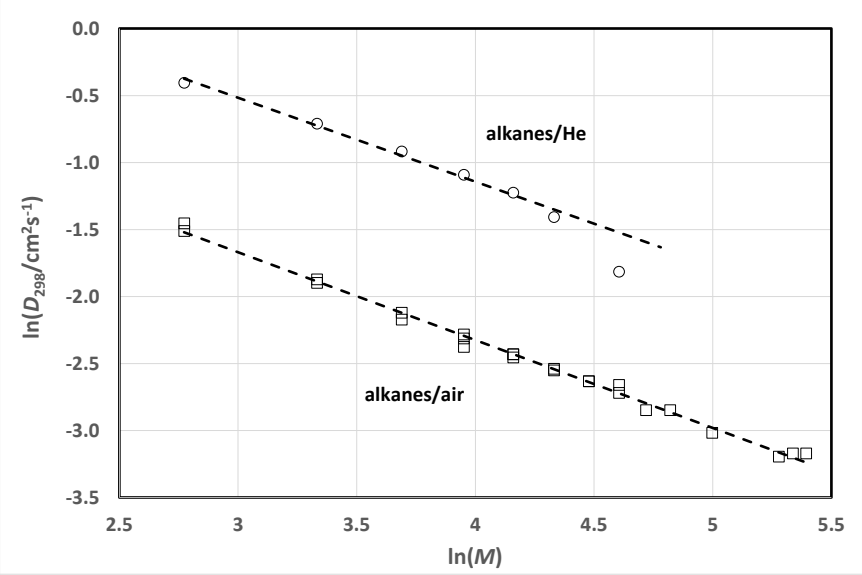

Figure 1. D_{298} for Alkanes as a Function of Mass in Air and Helium

We also find that as the compounds become more polar, that the barriers-to-diffusion (*E*) become higher – the following examples are for self-diffusion in the liquid phase (there are insufficient instances in the gas phase, but the correlation should be similar). In the table below, *n*-pentane, which is non-polar, has barrier of just 7 kJ mol^{-1} compared to 12 kJ mol^{-1} for the slightly polar benzene and toluene compared to the very polar *tert*-butanol which has a large barrier of 31 kJ mol^{-1}.

$$D = A \cdot e^{-E/RT}$$

Barriers-to-Diffusion by Compound Class (in the Liquid Phase)

Compound	*E*/kJ mol^{-1}	Ref.
n-pentane	6.93	31
n-hexane	8.22	31
ethyl acetate	10.8	32
toluene	12.1	34
benzene	12.3	33
octanoic acid	16.6	35
tert-pentanoic acid	20.3	34
tert-butanol	30.9	36

2.5. Details in Sources Regarding Diffusion Coefficients

In the evaluation of Ref. 3 by Tang *et al*., where the measurements in the literature were not carried out at 296 K, the original diffusivities were adjusted to 296 K using the relationship $D_{296} = D(T) \cdot (296/T)^{1.75}$. The diffusion coefficients in these tables from Ref. 7 by Gu *et al*. were taken from the original data in the supplementary information of that work, not from the tables in that paper (where there are some inconsistencies).

The diffusion coefficients from the sources where the diffusion coefficients were calculated from first principles (Refs. 10-31) were fit in the three ways outlined above: (1) $\ln(D) = A + B/T + C \cdot \ln(T)$ over the entire temperature range, (2) $D = A_n \cdot (T/298.15)^n$ over the entire temperature range, and (3) $\ln(D) = A + B/T$, which was fit just near room temperature to determine D_{298}.

3. Self- and Binaary-Diffusion Coefficients for Gases

Notation Used

Column Heading	Definition
Substance	atom or molecule
Bath	bath gas
T_{range}	reported temperature range, in K
T_{ref}	reference temperature (298 K or single temperature reported, see text), in K
D_{ref}	diffusion coefficient at reference temperature, in $cm^2\ s^{-1}$
U	expanded uncertainty in %
A	*A* coefficient in $\ln(D/cm^2\ s^{-1}) = A + B/(T/K) + C\cdot\ln(T/K)$
B	*B* coefficient in $\ln(D/cm^2\ s^{-1}) = A + B/(T/\,K) + C\cdot\ln(T/\,K)$
C	*C* coefficient in $\ln(D/cm^2\ s^{-1}) = A + B/(T/\,K) + C\cdot\ln(T/\,K)$
Ref	reference

The data in Table 1 is ordered by Chemical Compound Class and then by Molecular Formula.

Small Molecules	Hydrocarbons	Substituted Hydrocarbons
Rare gases	Alkanes (C-C)	Carbon-Oxygen species (CO/C(
Hydrogen-Oxygen species (H/(	Alkenes (C=C)	Alcohols (ROH)
Nitrogen compounds (N/H)	Alkynes (C#C)	Ethers (ROR)
NO_x compounds (N/H/O)	Cycloalkanes (-C..C-)	Ketones RC(O)R
Halogen compounds (H/X/O)	Alkylbenzenes (Ph-R)	Carboxylic acids (RCO_2H)
Sulfur compounds (S/H/O)	Polycyclic aromatics (PAHs)	Esters (RCO_2R)
		Nitrogen-substituted hydrocar
		Halogen-substituted hydrocarb

3.1.1. Table 1. Self- and Binary-Diffusion Coefficients for Gases

3.1.2. Table 1a. Small Molecules

Substance	Bath	T_{range}/K	T_{ref}/K	D_{ref}/ $cm^2\ s^{-1}$	*U*	*A*	*B*	*C*	Ref
Rare Gases									
He	He	77-888	298	1.759		-9.421	8.428	1.748	4
He	N_2	300-723	298	0.703	7.6%	-10.266	27.449	1.724	1
He	Ar	300-723	298	0.743	9.0%	-10.372	32.501	1.749	1
Ne	Ne	300-1400	298	0.511		-10.021	-9.327	1.647	4
Ar	He	300-723	298	0.728	6.8%	-9.843	1.729	1.671	1
Ar	Ar	235-418	298	0.182		-11.097	-45.486	1.676	4
Kr	Kr	70-5000	298	0.099	1-2%	-11.928	-38.548	1.709	19
Xe	Xe	100-5000	298	0.058	1-2%	-12.479	-50.933	1.721	20
Hydrogen-Oxygen									
H_2	H_2	115-295	298	1.309		-9.309	-8.028	1.686	4
D_2	D_2	195-353	298	0.933		-9.318	-1.746	1.624	4
OH	He	298	298	0.871					3
OH	Air	298	298	0.253					3
H_2O	N_2	150-2000	298	0.254	2-3%	-10.324	-84.181	1.620	25
H_2O	CO_2	250-2000	298	0.166	2-3%	-10.298	-180.060	1.597	27
D_2O	D_2O	250-2500	298	0.153	2-3%	-11.611	-189.247	1.817	22
O_2	O_2	55-2000	298	0.215	2-5%	-10.787	-44.220	1.649	29
HO_2	He	296	296	0.566					3
H_2O_2	Air	296	296	0.153					3
H_2O_2	Air	333	333	0.188					3
O_3	He	296	296	0.539					3
Nitrogen-Hydrogen									
NH_3	NH_3	301-446	298	0.190		0.811	-737.205	–	4
NH_3	N_2	293-523	298	0.227		-10.541	-60.256	1.625	3
NH_3	Air	298	298	0.228					3
NH_3	O_2	293-473	298	0.235		-10.882	-34.912	1.676	3
N_2	He	300-723	298	0.703	7.6%	-10.266	27.449	1.724	1
N_2	CH_4	70-1200	298	0.232	2-3%	-10.636	-48.119	1.637	16
N_2	H_2O	150-2000	298	0.254	2-3%	-10.324	-84.181	1.620	25
N_2	N_2	233-422	298	0.209		-10.397	-52.566	1.581	4
N_2	ethane	90-1200	298	0.154	2-4%	-10.945	-63.243	1.629	26
N_2	CO_2	253-473	298	0.224	1-3%	-7.317	-139.909	1.103	31
NO_x Species									
NO	N_2	293	293	0.232					3
NO	Air	296	296	0.232					3
N_2O	N_2O	150-1500		0.113	2.0%	-11.112	-112.381	1.635	17
NO_2	N_2	283	283	0.129					3
NO_2	Air	296	296	0.139					3
HONO	He	294	294	0.570					3
HONO	Air	296	296	0.126					3
NO_3	He	273	273	0.454					3
NO_3	N_2	273	273	0.105					3
NO_3	Air	296	296	0.121					3
NO_3	O_2	273	273	0.105					3

HNO_3	Air	296	296	0.120					3
$ClNO_2$	He	275	275	0.362					3
$ClNO_2$	N_2	275	275	0.099					3
$ClNO_2$	Air	296	296	0.112					3
N_2O_5	N_2	296	296	0.086					3
N_2O_5	Air	296	296	0.086					3
Halogen Species									
HCl	N_2	373-523	298	0.151		0.843	-814.331	–	3
HCl	Air	296	296	0.161					3
HCl	HCl	294.96	294.96	0.125					4
Cl_2	Air	296	296	0.124					3
HBr	N_2	391-525	298	0.122		0.438	-758.301	–	3
HBr	Air	296	296	0.125					3
HBr	HBr	295.26	295.26	0.079					4
HOBr	He	274	274	0.420					3
HOBr	N_2	274	274	0.111					3
HOBr	Air	296	296	0.111					3
HOI	He	253	253	0.296					3
Br_2	Air	298	298	0.107					3
ICl	He	293	293	0.389					3
I_2	N_2	273	273	0.070					3
I_2	Air	298	298	0.083					3
Sulfur Species									
H_2S	CH_4	150-1200	298	0.123		-11.160	-109.817	1.656	18
H_2S	ethane	150-1200	298	0.116		-11.324	-94.304	1.665	28
H_2S	H_2S	180-2000	298	0.119	1-2%	-11.287	-115.203	1.678	13
H_2S	CO_2	150-1200	298	0.182		-10.913	-75.475	1.660	18
SO_2	Air	296	296	0.124					3
SO_3	N_2	300	300	0.125					3
SO_3	Air	296	296	0.120					3
H_2SO_4	N_2	298	298	0.093					3
H_2SO_4	Air	296	296	0.097					3

3.1.3. Table 1b. Hydrocarbons

Substance	Bath	T_{range}/K	T_{ref}/K	D_{ref}/ $cm^2\ s^{-1}$	*U*	*A*	*B*	*C*	Ref
Alkanes									
CH_4	He	300-723	298	0.668	7.2%	-10.367	26.786	1.733	1
CH_4	CH_4	80-1500	298	0.232	2-6%	-10.725	-54.979	1.657	12
CH_4	N_2	250-500	298	0.234	1.1%	-10.325	-55.449	1.590	8
CH_4	Air	298	298	0.221					5
CH_4	Ethane	253-473	298	0.175	1-2%	-4.763	-350.286	0.737	31
CH_4	H_2S	150-1200	298	0.123		-11.160	-109.817	1.656	18
CH_4	CO_2	150-1200	298	0.182		-10.620	-86.243	1.615	18
CH_4	propane	150-1200	298	0.115	2-3%	-11.591	-63.882	1.692	20
ethane	He	300-723	298	0.492	12%	-10.690	29.230	1.735	2
ethane	CH_4	253-473	298	0.175	1-2%	-4.763	-350.286	0.737	31
ethane	N_2	300-723	298	0.154	13%	-10.064	-101.199	1.498	2
ethane	Air	298	298	0.150					5
ethane	Ethane	298-383	298	0.105		-0.069	-651.663	–	4
ethane	H_2S	150-1200	298	0.116		-11.324	-94.304	1.665	28
ethane	CO_2	297-625	298	0.115	4-6%	-10.582	-135.748	1.558	31
propane	He	300-723	298	0.400	12%	-11.063	44.904	1.755	2
propane	CH_4	150-1200	298	0.115	2-3%	-11.591	-63.882	1.692	20
propane	N_2	300-723	298	0.120	16%	-9.901	-131.167	1.442	2
propane	Air	298	298	0.114					5
propane	CO_2	150-1200	298	0.087	2-3%	-11.351	-107.782	1.628	20
propane	propane	160-1200	298	0.061	2-3%	-11.914	-111.570	1.668	21
propane	isobutane	298-626	298	0.051		-12.984	-54.058	1.787	31
n-butane	He	300-723	298	0.336	13%	-9.730	-50.409	1.546	2
n-butane	N_2	300-723	298	0.102	20%	-10.658	-96.357	1.526	2
methyl propane	Air	298	298	0.093					5
n-butane	Air	298	298	0.099					5
n-pentane	He	300-600	298	0.294	1.7%	-9.338	-60.094	1.460	6
n-pentane	N_2	350-600	298	0.088	7.6%	-9.732	-153.619	1.372	6
2,2-dimethyl propane	Air	298	298	0.088					5
n-pentane	Air	298	298	0.086					5
2,3-dimethyl butane	Air	298	298	0.079					5
2-methyl pentane	Air	298	298	0.093					5
n-hexane	Air	298	298	0.078					5
hexane	He	300-600	298	0.245	1.6%	-4.381	-387.669	0.750	6
2,4-dimethyl pentane	Air	298	298	0.072					5
n-heptane	Air	298	298	0.072					5
n-octane	He	350-600	298	0.163	3.6%	2.053	-890.802	-0.154	6
2,2,4-trimethyl pentane	Air	298	298	0.070					5
n-octane	Air	298	298	0.066					5
n-nonane	Air	298	298	0.058					5
2,3,3-trimethyl heptane	Air	298	298	0.068					5
n-decane	Air	298	298	0.058					5
n-dodecane	Air	298	298	0.049					5
n-hexadecane	Air	298	298	0.041					5
n-heptadecane	Air	298	298	0.042					5
n-octadecane	Air	298	298	0.042					5

Alkenes									
ethylene	ethylene	298-383	298	0.124		0.137	-662.037	–	4
ethylene	Air	298	298	0.163					5
propene	Air	298	298	0.132					5
1-butene	Air	298	298	0.109					5
cis-2-butene	Air	298	298	0.109					5
trans-2-butene	Air	298	298	0.109					5
1-pentene	Air	298	298	0.096					5
1-hexene	Air	298	298	0.080					5
2,3-dimethyl-2-butene	Air	298	298	0.080					5
1-octene	Air	298	298	0.064					5
Alkadienes									
propadiene	Air	298	298	0.139					5
1,3-butadiene	Air	298	298	0.116					5
2-methylbutadiene	Air	298	298	0.096					5
1,5-hexadiene	Air	298	298	0.080					5
2,3-dimethyl-1,3 -butadiene	Air	298	298	0.080					5
Alkynes									
acetylene	acetylene	298-383	298	0.131		0.607	-785.739	–	4
acetylene	Air	298	298	0.146					5
propyne	Air	298	298	0.132					5
1-butyne	Air	298	298	0.116					5
Cycloalkanes									
cyclopropane	Air	298	298	0.128					5
cyclopentane	Air	298	298	0.092					5
cyclohexane	Air	298	298	0.083					5
methylcyclopentane	Air	298	298	0.082					5
Alkylbenzenes									
benzene	H_2	311	311	0.404					9
benzene	He	423-523	298	0.285		1.320	-766.000	–	9
benzene	N_2	311	311	0.102					9
benzene	Air	298	298	0.095					5
benzene	O_2	311	311	0.101					9
benzene	Ar	323-373	298	0.070		-0.330	-693.000	–	9
benzene	toluene	331-692	298	0.027		-14.958	15.956	1.989	31
benzene	phenol	403-632	298	0.024		-14.020	-47.241	1.862	31
benzene	p-xylene	354-626	298	0.025		-14.273	-28.237	1.878	31
toluene	Air	298	298	0.088					5
ethyl benzene	Air	298	298	0.075					5
m-xylene	Air	298	298	0.068					5
o-xylene	Air	298	298	0.072					5
p-xylene	Air	298	298	0.067					5
1,2,4-trimethyl benzene	Air	298	298	0.064					5
1,3,5-trimethyl benzene	Air	298	298	0.066					5
isopropyl benzene	Air	298	298	0.067					5
n-propyl benzene	Air	298	298	0.067					5
p-isopropyltoluene	Air	298	298	0.063					5
p-tert-butyltoluene	Air	298	298	0.057					5
diphenyl	Air	298	298	0.068					5
Alkenylbenzenes									

styrene	Air	298	298	0.070					5
Polycyclic Aromatics									
naphthalene	H_2	303	303	0.301					9
naphthalene	Air	298	298	0.062					9
anthracene	Air	298	298	0.053					5

3.1.4. Table 1c. Oxidized Hydrocarbons

Substance	Bath	T_{range}/K	T_{ref}/K	D_{ref}/ $cm^2\ s^{-1}$	*U*	*A*	*B*	*C*	Ref
Carbon Oxides									
CO	CO	233-422	298	0.213		-10.132	-64.216	1.545	4
CO_2	CH_4	150-1200	298	0.182		-10.620	-86.243	1.615	18
CO_2	H_2O	250-2000	298	0.166	2-3%	-10.298	-180.060	1.597	27
CO_2	N_2	253-473	298	0.224	1-3%	-7.317	-139.909	1.103	31
CO_2	ethane	297-625	298	0.115	4-6%	-10.582	-135.748	1.558	31
CO_2	H_2S	150-1200	298	0.182		-10.913	-75.475	1.660	18
CO_2	CO_2	233-363	298	0.120		0.015	-637.089	–	4
CO_2	propane	150-1200	298	0.087	2-3%	-11.351	-107.782	1.628	20
Alcohols									
methanol	Air	298	298	0.166					5
methanol	trimethylamine	325-496	298	0.047		-13.730	-21.991	1.895	31
methanol	benzene	319-632	298	0.059		-13.255	-37.002	1.855	31
methanol	cyclohexane	316-630	298	0.053		-12.192	-121.829	1.702	31
ethanol	Air	298	298	0.129					5
1-propanol	Air	298	298	0.099					5
2-propanol	Air	298	298	0.104					5
1-butanol	Air	298	298	0.087					5
2-butanol	Air	298	298	0.088					5
1-pentanol	Air	298	298	0.071					5
2-pentanol	Air	298	298	0.071					5
1-hexanol	Air	298	298	0.062					5
2-ethyl-1-butanol	Air	298	298	0.066					5
1-heptanol	Air	298	298	0.055					5
1-octanol	Air	298	298	0.050					5
Alkanediols									
1,2-ethanediol	Air	298	298	0.100					5
1,2-propanediol	Air	298	298	0.088					5
Alkenols									
prop-2-en-1-ol	Air	298	298	0.103					5
Ethers									
diethyl ether	Air	298	298	0.092					5
diisopropyl ether	Air	298	298	0.068					5
di-*n*-butyl ether	Air	298	298	0.054					5
Cyclic Ethers									
ethylene oxide	ethylene oxide	200-1000	298	0.071	2.0%	-12.790	-102.290	1.832	14
1,4-dioxane	Air	298	298	0.092					5
Ketones									
acetone	Air	298	298	0.107					5
methyl ethyl ketone	Air	298	298	0.091					5
methyl *n*-propyl ketone	Air	298	298	0.079					5
Alkanoic Acids									
formic acid	Air	298	298	0.153					5
acetic acid	Air	298	298	0.124					5
propanoic acid	Air	298	298	0.095					5

2-methyl propanoic acid	Air	298	298	0.079					5
n-butanoic acid	Air	298	298	0.078					5
3-methyl butanoic acid	Air	298	298	0.066					5
4-methyl pentanoic acid	Air	298	298	0.059					5
hexanoic acid	Air	298	298	0.061					5
Esters									
methyl formate	Air	298	298	0.109					5
ethyl formate	Air	298	298	0.100					5
propyl formate	Air	298	298	0.083					5
2-methylpropyl formate	Air	298	298	0.079					5
isopentyl formate	Air	298	298	0.067					5
n-pentyl formate	Air	298	298	0.066					5
methyl acetate	Air	298	298	0.112					5
ethyl acetate	Air	298	298	0.088					5
propyl acetate	Air	298	298	0.076					5
2-methylpropyl acetate	Air	298	298	0.068					5
n-butyl acetate	Air	298	298	0.067					5
n-pentyl acetate	Air	298	298	0.061					5
benzyl acetate	Air	298	298	0.061					5
methyl propanoate	Air	298	298	0.087					5
ethyl propanoate	Air	298	298	0.080					5
isobutyl propanoate	Air	298	298	0.061					5
n-butyl propanoate	Air	298	298	0.061					5
n-pentyl propanoate	Air	298	298	0.055					5
methyl *n*-butanoate	Air	298	298	0.075					5
ethyl isobutanoate	Air	298	298	0.067					5
ethyl n-butanoate	Air	298	298	0.067					5
isopropyl isobutanoate	Air	298	298	0.063					5
isobutyl isobutanoate	Air	298	298	0.055					5
methyl *n*-pentanoate	Air	298	298	0.067					5
ethyl n-pentanoate	Air	298	298	0.061					5
methyl hexanonate	Air	298	298	0.061					5

3.1.5. Table 1d. Nitrogen-Substituted Hydrocarbons

Substance	Bath	T_{range}/K	T_{ref}/K	D_{ref}/ $cm^2\ s^{-1}$	*U*	*A*	*B*	*C*	Ref
Alkyl Amines									
diethylamine	Air	298	298	0.099					5
isobutylamine	Air	298	298	0.089					5
n-butylamine	Air	298	298	0.087					5
triethylamine	Air	298	298	0.075					5
Cycloamines									
piperidine	Air	298	298	0.087					5
Nitriles									
HCN	Air	298	298	0.201					5
2-propenenitrile	Air	298	298	0.105					5
benzonitrile	Air	298	298	0.071					5
N-substituted Aromatics									
pyridine	Air	298	298	0.095					5
aniline	Air	298	298	0.074					5
nitrobenzene	Air	298	298	0.079					5

3.1.6. Table 1e. Halogen-Substituted Hydrocarbons

Substance	Bath	T_{range}/K	T_{ref}/K	D_{ref}/ $cm^2\ s^{-1}$	*U*	*A*	*B*	*C*	Ref
Fluorocarbons									
fluoromethane	N_2	300-550	298	0.184	1.3%	-11.647	-12.790	1.755	8
difluoromethane	N_2	300-650	298	0.155	1.5%	-11.617	-16.745	1.721	8
trifluoromethane	N_2	300-723	298	0.144	1.9%	-12.178	30.366	1.780	8
tetrafluoromethane	CH_4	298-383	298	0.122		-0.066	-607.505	–	7
fluorobenzene	Air	295	295	0.083					7
Chloroalkanes									
chloromethane	CH_4	298-478	298	0.143		0.456	-715.306	–	7
chloromethane	Air	298	298	0.143					7
chloroethane	chloromethane	358-438	298	0.054		-0.088	-842.964	–	7
dichloromethane	He	298	298	0.104					7
1-chlorobutane	Air	296	296	0.090					7
1,2-dichloroethane	Air	295	295	0.090					7
1,2-dichloroethane	Air	298	298	0.092					7
trichloromethane	N_2	383-418	298	0.077		0.260	-843.020	–	7
trichloromethane	Air	298-328	298	0.091		-0.647	-522.355	–	7
trichloromethane	CO_2	363-383	298	0.079		-0.670	-556.413	–	7
1,1,1-trichloroethane	Air	298	298	0.079					7
1,1,2-trichloroethane	Air	298	298	0.079					7
tetrachloromethane	N_2	364-423	298	0.074		-0.308	-682.285	–	7
tetrachloromethane	Air	298-348	298	0.078		-0.632	-573.918	–	7
tetrachloromethane	CO_2	363-423	298	0.058		-0.691	-643.778	–	7
1,1,2,2-tetrachloroethane	Air	298	298	0.072					7
pentachloroethane	Air	298	298	0.067					7
Chloroalkenes									
chloroethylene	Air	298	298	0.122					7
1,2-dichloroethylene	Air	298	298	0.114					7
trichloroethylene	Air	298	298	0.088					7
tetrachloroethylene	Air	298	298	0.080					7
Aromatic Chlorocarbons									
chlorobenzene	Air	299-332	298	0.073		-0.649	-587.718	–	7
2-chlorotoluene	Air	298	298	0.068					7
3-chlorotoluene	Air	298	298	0.064					7
4-chlorotoluene	Air	298	298	0.062					7
benzyl chloride	Air	298	298	0.071					7
Bromocarbons									
bromoethane	Air	296	296	0.106					7
1-bromopropane	Air	298	298	0.088					7
1-bromobutane	N_2	303	303	0.080					7
1,2-dibromoethane	Air	298	298	0.083					7
tribromomethane	Air	298	298	0.076					7
Iodocarbons									
iodoethane	Air	295	295	0.098					7
1-iodopropane	N_2	303	303	0.079					7
1-iodopropane	Air	298	298	0.087					7
Chlorofluorocarbons									
dichlorodifluoromethane	H_2O	298	298	0.105					7

dichlorodifluoromethane	Air	298	298	0.095					7
Bromochlorocarbons									
bromochloromethane	Air	298	298	0.095					7
Oxidized Chlorocarbons									
CCl_2O	Air	273	273	0.095					7

4. Summary

In summary, we have compiled, evaluated, and recommend self-diffusion and binary-diffusion coefficients *D* for gases at standard room temperature 298.15 K (D_{298}) and standard atmospheric pressure (101.325 kPa). We also provided recommended expressions for many diffusion coefficients as a function of temperature, where the data was available in the literature. We provided approximately 270 binary-diffusion coefficients with ~200 in air, N_2, or O_2, and ~20 in helium (the remainder in other bath gases), and approximately 25 self-diffusion coefficients. These diffusion coefficients are for compounds in roughly 35 different chemical classes consisting of rare gases, small H/O/N/S species, hydrocarbons, and oxygen-, nitrogen-, and halogen-substituted hydrocarbons.

Declaration of Competing Interest

The authors have no conflicts to disclose.

Data Availability

The data that support the findings of this study are available within the article.

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