# Supporting information for "Compilation and evaluation of gas phase diffusion coefficients of halogenated organic compounds"

Instruction:

1. Units used in this work is K for temperature ($T$) and Torr for pressure ($P$).

2. Experimentally measured diffusion coefficients reported in literature have been converted to measured diffusivities ($D_m$) in the unit of Torr $cm^2$ $s^{-1}$, and Fuller's semi-empirical method is used in this work to estimate diffusivities ($D_e$, in the unit of Torr $cm^2$ $s^{-1}$).

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# 1 Compounds with one carbon atom

## 1.1 $CH_3Cl$

| bath gas | reference. | *T* | *P* | *D*m | *D*e | (*D*m-*D*e)/*D*e (%) |
|---|---|---|---|---|---|---|
| air | [1] | 298 | 760 | 109±2 | 99 | 10 |
| $CH_4$ | [2] | 298 | 740 | 108 | 113 | -4 |
| | | 358 | 739 | 154 | 156 | -1 |
| | | 418 | 745 | 208 | 205 | 2 |
| | | 478 | 735 | 267 | 258 | 3 |
| | | 298 | 739 | 107 | 113 | -5 |
| | | 378 | 743 | 171 | 172 | -1 |
| | | 438 | 733 | 228 | 222 | 3 |
| $SO_2$ | [3] | 303 | 760 | 53 | 65 | -19 |
| | | 313 | 760 | 56 | 69 | -19 |
| | | 323 | 760 | 58 | 73 | -20 |
| | | 333 | 760 | 63 | 77 | -18 |
| $CH_3OCH_3$ | [3] | 303 | 760 | 51 | 66 | -21 |
| | | 313 | 760 | 55 | 69 | -21 |
| | | 323 | 760 | 57 | 73 | -22 |
| | | 333 | 760 | 62 | 77 | -20 |

The diffusivity of $CH_3Cl$ in air at 298 K was measured by Cowie and Watts,[1] and the measured diffusivity is 10% larger than the estimated value.

Gotoh et al. measured the diffisitivities of $CH_3Cl$ in $CH_4$ from 298 to 438 K,[2] and the differences between the measured and estimated diffusivities are <5% across the entire temperature range.

The diffusitivities of $CH_3Cl$ in $SO_2$ and $CH_3OCH_3$, measured by Chakraborti and Gray,[3] are around 20% smaller than estimated values for temperatures in the range of 303 to 333 K.

**References:**

[1] Cowie, M., and Watts, H.: Diffusion of methane and chloromethanes in air, ***Canadian Journal of Chemistry,*** 49, 74-77, 1971.

[2] Gotoh, S., Manner, M., Sorensen, J. P., and Stewart, W. E.: Binary diffusion-coefficients of low-density gases .1. Measurements by modifide loschmidt method, ***J. Chem. Eng. Data***, 19, 169-171, 1974.

[3] Chakraborti, P. K., and Gray, P.: Diffusion coefficients in binary mixtures of polar gas-sulphur dioxide, dimethtl ether and methyl chlorine, ***Transactions of the Faraday Society***, 62, 3331-3337, 1966.

### 1.2 $CH_3I$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 431 | 760 | 595±12 | 602 | -1 |

The diffusivity of $CH_3I$ in He, measured at 431 K by Fuller et al.,[1] is only 1% smaller than the estimated value.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

### 1.3 $CH_2F_2$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 431 | 760 | 664±23 | 633 | 5 |

The diffusivity of $CH_2F_2$ in He, measured at 431 K by Fuller et al.,[1] is 5% laregr than the estimated value.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

### 1.4 $CH_2Cl_2$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 428 | 760 | 570±7 | 552 | 3 |
| air | [2] | 298 | 760 | 79±4 | 79 | 0 |
| | [3] | 298 | 760 | 79±4 | 79 | -1 |
| | [4] | 288 | 760 | 76 | 75 | 1 |
| | | 298 | 760 | 79 | 80 | 0 |
| | | 308 | 760 | 83 | 84 | -1 |
| Kr | [5] | 278 | 16 | 39 | 48 | -17 |
| | | 288 | 18 | 42 | 50 | -17 |
| | | 303 | 21 | 47 | 55 | -15 |
| | | 318 | 24 | 51 | 60 | -15 |

The diffusivity of $CH_2Cl_2$ in He at 428 K, measured Fuller et al.,[1] is 3% larger than the estimated value.

The diffusivities of $CH_2Cl_2$ in air, measured at 298 K by Cowie and Watts [2] and by Lugg [3] and from 288 to 308 K by Watts,[4] show excellent agreement with estimated values, with difference being 1% or smaller.

The diffusivities of $CH_2Cl_2$ in Kr, measured by Singh and Srivastava from 278 to 318 K,[5] are 15% to 17% smaller than the estimated values.

**References:**


[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Cowie, M., and Watts, H.: Diffusion of methane and chloromethanes in air, ***Canadian Journal of Chemistry***, 49, 74-77, 1971.

[3] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

[4] Watts, H.: Temperature dependence of diffusion of carbon tetrachloride, chloroform and methylene chloride vapors in air by a rate of evaporation method, ***Canadian Journal of Chemistry***, 49, 67-73, 1971.

[5], B. N.: Unlike interactions and binary diffusion in polar-nonpolar mixtures-krypton-methylene chloride and krypton-ethylchloride, ***International Journal of Heat and Mass Transfer***, 11, 1771-1778, 1968.

### 1.5 $CH_2ClBr$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| air | [1] | 298 | 760 | 72±1 | 81 | -10 |

The measured diffusivity of $CH_2ClBr$ in air at 298 K [1] is 10% smaller than the estimated value.

**References:**

[1] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

### 1.6 $CH_2Br_2$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 428 | 760 | 505±5 | 550 | -8 |

The measured diffusivity of $CH_2Br_2$ in He at 428 K [1] is 8% smaller than the estimated value.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

### 1.7 $CHCl_3$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 429 | 760 | 474±9 | 483 | -2 |
| $N_2$ | [2] | 361 | 760 | 103 | 99 | 3 |
| | | 383 | 760 | 109 | 110 | -1 |
| | | 403 | 760 | 122 | 120 | 2 |
| | | 418 | 760 | 131 | 128 | 3 |
| air | [3] | 308 | 760 | 77 | 73 | 5 |
| | [4] | 298 | 760 | 67±1 | 69 | -2 |
| | [5] | 323 | 760 | 83±2 | 79 | 5 |
| | [6] | 298 | 760 | 66±1 | 69 | -5 |
| | [7] | 298 | 760 | 69 | 69 | 0 |
| | | 308 | 760 | 73 | 73 | 0 |
| | | 318 | 760 | 77 | 77 | 0 |
| | | 328 | 760 | 81 | 81 | 0 |
| $CO_2$ | [2] | 363 | 760 | 84 | 76 | 10 |
| | | 383 | 760 | 91 | 84 | 9 |
| | | 404 | 760 | 98 | 92 | 7 |
| Kr | [8] | 284 | 11 | 36 | 41 | -12 |
| | | 293 | 11 | 38 | 43 | -13 |
| | | 303 | 13 | 41 | 46 | -12 |
| | | 313 | 13 | 43 | 49 | -12 |
| $C_2H_5OC_2H_5$ | [9] | 293 | 760 | 22 | 30 | -25 |

The diffusivity of $CHCl_3$ in He at 429 K, measured by Fuller et al.,[1] is 2% smaller than the estimated value.

Nagata and Hasegawa investigated the temperature dependence of diffusivities of $CHCl_3$ in $N_2$ from 361 to 418 K,[2] and differences between the measured and estimated values are not larger than 3%.

Five studies measured the diffusivities of $CHCl_3$ in air at different temperatures from 298 to 328 K.[3-7] Differences between the measured and estimated diffusivities are around 5% or smaller.

Nagata and Hasegawa measured the diffusivities of $CHCl_3$ in $CO_2$ at 363, 383, and 404 K.[2] The differences between the measured and estimated diffusivities are around 10% or smaller.

Srivastava and Saran measured the diffusivities of $CHCl_3$ in Kr at 284, 293, 303, and 313 K,[8] and the measured diffusivities are around 13% smaller than the estimated values.

The diffusivity of $CHCl_3$ in $C_2H_5OC_2H_5$ at 293 K, measured by Weissman,[9] is 25% smaller than the estimated value.

**References:**


[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, ***J. Chem. Engng. Japan,*** 3, 143-145, 1970.

[3] Getzinger, R. W., and Wilke, C. R.: An experimental study of nonequimolal diffusion in ternary gas mixtures, ***Aiche J.***, 13, 577-580, 1967.

[4] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

[5] Mrazek, R. V., Wicks, C. E., and Prabhu, K. N. S.: Dependence of diffusion coefficient on composition in binary gaseous systems, ***J. Chem. Eng. Data***, 13, 508-510, 1968.

[6] Cowie, M., and Watts, H.: Diffusion of methane and chloromethanes in air, ***Canadian Journal of Chemistry***, 49, 74-77, 1971.

[7] Watts, H.: Temperature dependence of diffusion of carbon tetrachloride, chloroform and methylene chloride vapors in air by a rate of evaporation method, ***Canadian Journal of Chemistry***, 49, 67-73, 1971.

[8] Srivastava, B. N., and Saran, A.: Mutual diffusion studies in krypton-acetone and krypton-chloroform systems, ***Physica***, 32, 110-118, 1966.

[9] Weissman, S.: Estimation of diffusion coefficients from viscosity measurements-polar + polyatomic gases, ***J. Chem. Phys.***, 40, 3397-3406, 1964.

### 1.8 $CHBr_3$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| air | [1] | 298 | 760 | 58±1 | 71 | -18 |

The measured diffusivity of $CHBr_3$ in air at 298 K [1] is 18% smaller than the estimated value.

**References:**

[1] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

### 1.9 $CF_2Cl_2$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| air | [1] | 298 | 760 | 72±3 | 67 | 7 |
| $H_2O$ | [2] | 298 | 760 | 80 | 90 | -11 |
| ethanol | [2] | 298 | 760 | 36 | 43 | -15 |
| benzene | [2] | 298 | 760 | 29 | 28 | 4 |
| di-n-butyl phthalate | [3] | 293 | 760 | 9.6 | 13.5 | -29 |
| | | 303 | 760 | 10.6 | 14.3 | -26 |

The differences between the measured diffusivity of $CF_2Cl_2$ in air,[1] $H_2O$,[2] ethanol,[2] and benzene [2] at 295 K and estimated values are 7%, 11%, 14%, and 4%, respectively.

Briks et al.[3] measurd the diffusivities of $CF_2Cl_2$ in di-n-butyl phthalate at 293 and 303 K, and the measured diffusivities are 29% and 26% smaller than the measured values.

**References:**


[1] Barr, R. F., and Watts, H.: Diffusion of some organic and inorganic compounds in air, ***J. Chem. Eng. Data***, 17, 45-46, 1972.

[2] Lee, C. Y., and Wilke, C. R.: Measurements of vapor diffusion coefficient, ***Industrial and Engineering Chemistry***, 46, 2381-2387, 1954.

[3] Birks, J., and Bradley, R. S.: The rate of evaporation od droplets. 2. the influence of changes of temperature and of the surrounding gas on the rate of evaporation of drops of di-normal-butyl phthalate, ***Proceedings of the Royal Society of London Series a-Mathematical and Physical Sciences***, 198, 226-239, 1949.

### 1.10 $CF_4$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| $CH_4$ | [1] | 298 | 760 | 92.7 | 87.6 | 6 |
| | | 353 | 760 | 126.9 | 117.5 | 8 |
| | | 383 | 760 | 145.9 | 135.5 | 8 |
| $SF_6$ | [2] | 303 | 760 | 36.3 | 32.7 | 11 |
| | | 313 | 760 | 38.5 | 34.6 | 11 |
| | | 329 | 760 | 42.1 | 37.8 | 12 |
| | | 342 | 760 | 45.2 | 40.4 | 12 |
| n-hexane | [3] | 283 | 760 | 29.6 | 26.6 | 11 |
| | | 298 | 760 | 33.1 | 29.1 | 13 |
| | | 313 | 760 | 36.6 | 31.8 | 15 |
| | | 328 | 760 | 39.7 | 34.5 | 15 |
| cyclohexane | [4] | 283 | 760 | 30.9 | 27.1 | 14 |
| | | 298 | 760 | 33.7 | 29.7 | 14 |
| | | 313 | 760 | 37.3 | 32.4 | 15 |
| | | 328 | 760 | 40.2 | 35.1 | 14 |
| | | 343 | 760 | 43.6 | 38.0 | 15 |
| benzene | [4] | 283 | 760 | 34.7 | 30.8 | 13 |
| | | 298 | 760 | 37.5 | 33.7 | 11 |
| | | 313 | 760 | 42.1 | 36.7 | 15 |
| | | 328 | 760 | 45.4 | 39.9 | 14 |
| | | 343 | 760 | 49.2 | 43.1 | 14 |
| n-heptane | [3] | 283 | 760 | 28.5 | 24.3 | 17 |
| | | 298 | 760 | 29.4 | 26.6 | 11 |
| | | 313 | 760 | 32.3 | 29.0 | 11 |
| | | 328 | 760 | 35.7 | 31.5 | 14 |
| | | 343 | 760 | 38.3 | 34.0 | 13 |
| methylcyclohexane | [4] | 283 | 760 | 25.9 | 24.7 | 5 |
| | | 298 | 760 | 29.2 | 27.0 | 8 |
| | | 313 | 760 | 33.7 | 29.5 | 14 |
| | | 328 | 760 | 36.1 | 32.0 | 13 |
| | | 343 | 760 | 39.2 | 34.6 | 13 |

| | | | | | | |
|---|---|---|---|---|---|---|
| toluene | [4] | 283 | 760 | 29.4 | 27.5 | 7 |
| | | 298 | 760 | 33.1 | 30.1 | 10 |
| | | 313 | 760 | 36.6 | 32.8 | 11 |
| | | 328 | 760 | 40.0 | 35.6 | 12 |
| | | 343 | 760 | 43.9 | 38.5 | 14 |
| octane | [3] | 283 | 760 | 20.9 | 22.5 | -7 |
| | | 283 | 760 | 24.1 | 22.5 | 7 |
| | | 298 | 760 | 27.4 | 24.6 | 12 |
| | | 298 | 760 | 27.7 | 24.6 | 12 |
| | | 313 | 760 | 31.8 | 26.8 | 19 |
| | | 313 | 760 | 29.6 | 26.8 | 11 |
| | | 328 | 760 | 33.1 | 29.1 | 14 |
| | | 328 | 760 | 32.7 | 29.1 | 12 |
| | | 343 | 760 | 35.2 | 31.5 | 12 |
| | | 343 | 760 | 34.4 | 31.5 | 9 |

Mueller and Cahill [1] measured the diffusivities of $CF_4$ in $CH_4$ from 298-383 K, and the differences between the measured and estimated diffusivities are around 8% or smaller.

Raw and Tang [2] measured the diffusivities of $CF_4$ in $SF_6$ from 303 to 342 K, and the differences between the measured and estimated diffusivities are around 12%.

Wilhelm and Battino [3] measured the diffusivities of $CF_4$ in n-haxane from 283 to 328 K, and the measuered diffusivities are 11% to 15% larger than the estimated values.

Wilhelm et al. [4] measured the diffusivities of $CF_4$ in cyclohaxane from 283 to 343 K, and the measured diffusivities are ~15% larger than the estimated values.

The diffusivities of $CF_4$ in benzene are measuered by Wilhelm from 283 to 343 K,[4] and the differences between the measured and estimated diffusivities are around 15% or smaller.

Wilhelm and Battino [3] measured the diffusivities of $CF_4$ in n-heptane from 283 to 343 K, and the differences between the measured and estimated diffusivities are 17% or smaller.

Wilhelm et al.[4] measured the diffusivities of $CF_4$ in methylcyclohexane from 283 to 343 K, and the measured diffusivities are 5% to 14% larger than the estimated values.

Wilhelm et al.[4] measured the diffusivities of $CF_4$ in toluene from 283 to 343 K, and the differences between the measured and estimated values are 14% or smaller.

Wilhelm and Battino [3] measured the diffusivities of $CF_4$ in octane from 283 to 343 K, and the difference between the measured and estimated diffusivities are 19% or smaller.

**References:**


[1] Mueller, C. R., and Cahill, R. W.: Mass spectrometric measurement of diffusion coefficients, ***J. Chem. Phys.***, 40, 651-654, 1964.

[2] Raw, C. J. G., and Tang, H.: Viscosity and diffusion coefficients of gaseous sulfur hexafluoride-carbon tetrafluoride mixtures, ***J. Chem. Phys.***, 39, 2616-2618, 1963.

[3] Wilhelm, E., and Battino, R.: Binary gaseous diffusion-coefficients .1. methane and carbon tetrafluoride with hexane, heptane, octane, and 2,2,4-trimethylpentane at one-atmosphere pressure at 10-70 degrees c, ***J. Chem. Eng. Data***, 17, 187-189, 1972.

[4] Wilhelm, E., Battino, R., and Carpente.Rl: Binary gaseous diffusion-coefficients .2. methane and carbon tetrafluoride with cyclohexane, methylcyclohexane, benzene, and toluene at 1atm at 10-70 degrees c, ***J. Chem. Eng. Data***, 19, 245-246, 1974.

### 1.11 $CCl_4$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| $N_2$ | [1] | 364 | 760 | 86 | 90 | -5 |
| | | 383 | 760 | 94 | 99 | -5 |
| | | 403 | 760 | 102 | 108 | -6 |
| | | 423 | 760 | 112 | 117 | -5 |
| | [2] | 353 | 760 | 84 | 86 | -2 |
| air | [3] | 298 | 760 | 63±1 | 62 | 2 |
| | [4] | 298 | 760 | 58±1 | 62 | -7 |
| | [5] | 308 | 760 | 68 | 65 | 4 |
| | [6] | 295 | 740 | 58 | 61 | -5 |
| | | 296 | 743 | 57 | 61 | -6 |
| | [7] | 298 | 760 | 59 | 62 | -5 |
| | | 308 | 760 | 63 | 65 | -4 |
| | | 318 | 760 | 66 | 69 | -4 |
| | | 328 | 760 | 70 | 73 | -4 |
| | | 338 | 760 | 74 | 77 | -4 |
| | | 348 | 760 | 78 | 81 | -4 |
| | [8] | 295 | 762 | 61 | 61 | 1 |
| | [9] | 313 | 760 | 67 | 67 | 1 |
| $CO_2$ | [1] | 363 | 760 | 65 | 68 | -5 |
| | | 384 | 760 | 71 | 75 | -6 |
| | | 403 | 760 | 76 | 82 | -7 |
| | | 423 | 760 | 84 | 89 | -5 |
| benzene | [10] | 293 | 760 | 19±1 | 17 | 12 |
| $CH_2Cl_2$ | [10] | 293 | 760 | 22±1 | 29 | -26 |
| | | 353 | 760 | 32±1 | 40 | -21 |
| | | 413 | 760 | 42±4 | 53 | -22 |
| $CHCl_3$ | [10] | 293 | 760 | 20±1 | 24 | -17 |

The diffusivities of $CCl_4$ in $N_2$ were measured by Nagata and Hasegawa [1] from 364 to 423 K and by Arinikar [2] at 353 K. The measured diffusivities are 2% to 6% smaller than the estimated values.

Five studies measured the diffusivities of $CCl_4$ in air at 295-298 K,[3, 4, 6-8] and the differences between the measured and estimated diffusivities are 7% or smaller. Getzinger and Wilke [5] and Richardson [9] measured the diffusivities of $CCl_4$ in air at 308 and 313 K, and the differences between the measured and estimated values are 4% or smaller. The temperature dependence of diffusivities of $CCl_4$ in air was investigated from 298 to 348 K by Watts.[7] The differences between the measured and estimated diffusivities are 5% or smaller across the entire temperature range investigated.

Nagata and Hasegawa [1] measured the diffusivities of $CCl_4$ in $CO_2$ from 363 to 423 K, and the measured diffusivities are around 6% smaller than the estimated values.

Weissman [10] measured the diffusivity of $CCl_4$ in benzene at 293 K, and the measured diffusivity is 12% larger than the estimated value.

Weissman [10] measured the diffusivities of $CCl_4$ in $CH_2Cl_2$ at 293, 353, and 413 K, and the measured diffusivities are all around 25% smaller than estimated values.

The diffusivity of $CCl_4$ in $CHCl_3$ was measured by Weissman at 293 K,[10] and the measured diffusivity is 17% smaller than the estimated value.

**References:**


[1] Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, ***J. Chem. Engng. Japan***, 3, 143-145, 1970.

[2] Arnikar, H. J., Rao, T. S., and Karmarkar, K. H.: Eletrodeless discharge as detector in gas chromatography. 3. study of inter-diffusion of gases, ***International Journal of Electronics***, 22, 381-385, 1967.

[3] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

[4] Cowie, M., and Watts, H.: Diffusion of methane and chloromethanes in air, ***Canadian Journal of Chemistry***, 49, 74-77, 1971.

[5] Getzinger, R. W., and Wilke, C. R.: An experimental study of nonequimolal diffusion in ternary gas mixtures, ***Aiche J.***, 13, 577-580, 1967.

[6] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, ***Journal of Heat Transfer***, 91, 259-265, 1969.

[7] Watts, H.: Temperature dependence of diffusion of carbon tetrachloride, chloroform and methylene chloride vapors in air by a rate of evaporation method, ***Canadian Journal of Chemistry***, 49, 67-73, 1971.

[8] Pryde, J. A., and Pryde, E. A.: A simple quantitative diffusion experiment, ***Physics Education***, 2, 311-314, 1967.

[9] Richardson, J. F.: The evaporation of two-component liquid mixtures, ***Chem. Eng. Sci.***, 10, 234-242, 1959.

[10] Weissman, S.: Estimation of diffusion coefficients from viscosity measurements-polar + polyatomic gases, ***J. Chem. Phys.***, 40, 3397-3406, 1964.

### 1.12 $CCl_2O$, $CCl_3NO_2$, and CNCl

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CCl_2O$ | air | [1] | 273 | 760 | 72 | 66 | 9 |
| $CCl_3NO_2$ | air | [1] | 298 | 760 | 67 | 63 | 7 |
| | | [2] | 298 | 760 | 62±1 | 63 | -2 |
| CNCl | air | [1] | 273 | 760 | 84 | 84 | 1 |

The measured diffusivities in air are 9% larger than the estimated value for $CCl_2O$ and 1% larger for CNCl.[1]

Two studies measured the diffusivities of $CCl_3NO_2$ in air at 298 K, and the measured values are 7% larger [1] and 2% smaller [2] than the estimated ones.

**References:**

[1] Klotz, I. M., and Miller, D. K.: Diffusion coefficients and molecular radii of hydrogen cyanide, cyanogen chloride, phosgene and chloropicrin, J. Am. Chem. Soc., 69, 2557-2558, 1947.

[2] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, Analytical Chemistry, 40, 1072-1077, 1968.

# 2 Compounds with two carbon atoms

## 2.1 $CH_3CH_2Cl$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| $CH_3Cl$ | [1] | 298 | 731 | 43 | 54 | -22 |
| | | 298 | 736 | 42 | 55 | -22 |
| | | 358 | 742 | 64 | 75 | -14 |
| | | 378 | 741 | 74 | 83 | -10 |
| | | 419 | 741 | 90 | 99 | -9 |
| | | 438 | 731 | 98 | 107 | -9 |
| Kr | [2] | 275 | 21 | 45 | 50 | -9 |
| | | 288 | 28 | 55 | 54 | 2 |
| | | 303 | 21 | 54 | 59 | -7 |
| | | 318 | 24 | 60 | 64 | -6 |

Gotoh et al.[1] measured the diffusivities in $CH_3Cl$ from 298 to 438 K, and the differences between the measured and estimated diffusivities are around 22% or less.

The diffusivities of $CH_3CH_2Cl$ in Kr were measured from 275 to 318 K by Singh and Srivastava,[2] and the differences between the measured and estimated diffusivitiies are smaller than 10%.

**References:**


[1] Gotoh, S., Manner, M., Sorensen, J. P., and Stewart, W. E.: Binary diffusion-coefficients of low-density gases .1. Measurements by modifide loschmidt method, ***J. Chem. Eng. Data***, 19, 169-171, 1974.

[2] Singh, Y., and Srivastava, B. N.: Unlike interactions and binary diffusion in polar-nonpolar mixtures-krypton-methylene chloride and krypton-ethylchloride, ***International Journal of Heat and Mass Transfer***, 11, 1771-1778, 1968.

## 2.2 $CH_3CH_2Br$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 428 | 760 | 562±8 | 548 | 3 |
| Air | [2] | 298 | 760 | 75±1 | 84 | -11 |
| | [3] | 295 | 745 | 80 | 83 | -4 |
| | | 295 | 729 | 79 | 83 | -5 |
| | | 296 | 736 | 78 | 83 | -6 |

The diffusivity of $CH_3CH_2Br$ in He at 428 K, measured by Fuller et al.,[1] is 3% larger than the estimated value.

Lugg [2] and Grob and Elwakil [3] measurd the diffusivities of $CH_3CH_2Br$ in air at around room temperature, and the differences between measured and estimated diffusivities are 4% to 6%.

**References:**


[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

[3] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, ***Journal of Heat Transfer***, 91, 259-265, 1969.

### 2.3 $CH_3CH_2I$

| bath gas | reference | T | P | Dm | De | (Dm-De)/De |
|---|---|---|---|---|---|---|
| air | [1] | 295 | 736 | 72 | 69 | 4 |
| | | 295 | 730 | 72 | 69 | 4 |
| | | 295 | 737 | 71 | 69 | 3 |
| He | [2] | 428 | 760 | 492±10 | 506 | -3 |

The average diffusivity of $CH_3CH_2I$ in air at 295 K, measured by Grob and Elwakil,[1] is ~3% larger then the estimated value.

The diffusivity of $CH_3CH_2I$ in He at 428 K, measured by Fuller et al.,[2] is 3% smaller than the estimated value.

**References:**

[1] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, ***Journal of Heat Transfer***, 91, 259-265, 1969.

[2] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

## 2.4 $CH_3CHF_2$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 430 | 760 | 573±11 | 527 | 9 |

The diffusivity in He at 430 K, measured by Fuller et al.,[1] is 9% larger than the estimated value.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

## 2.5 $CH_2ClCH_2Cl$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 427 | 760 | 519±5 | 476 | 9 |
| air | [2] | 295 | 745 | 67 | 68 | -2 |
| | | 295 | 738 | 67 | 68 | -1 |
| | | 295 | 742 | 66 | 68 | -4 |
| | [3] | 298 | 760 | 70±1 | 70 | 0 |
| | | 298 | 760 | 69±1 | 70 | -1 |

The diffusivity of $CH_2ClCH_2Cl$ in He at 427 K, measured by Fuller et al.,[1] is 9% larger than the estimated value.

The diffusivities of $CH_2ClCH_2Cl$ in air were measured by two studies at around room temperature,[2,3] and the differences between the measured and estimated values are 4% or less.

**References:**


[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, ***Journal of Heat Transfer***, 91, 259-265, 1969.

[3] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

## 2.6 $CH_2BrCH_2Br$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m\text{-}De)/D_e$ (%) |
|---|---|---|---|---|---|---|
| air | [1] | 298 | 760 | 63±1 | 72 | -13 |

The diffusivity of $CH_2BrCH_2Br$ in air at 298 K, measured by Lugg,[1] is 13% smaller than the estimated value.

**References:**

[1] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

## 2.7 $CCl_3CH_3$ and $CHCl_2CH_2Cl$

| species | reference | bath gas | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CCl_3CH_3$ | [1] | air | 298 | 760 | 60±1 | 62 | -2 |
| $CHCl_2CH_2Cl$ | [1] | air | 298 | 760 | 60±1 | 62 | -2 |

Lugg [1] measured the diffusivities of $CCl_3CH_3$ and $CHCl_2CH_2Cl$ in air at 298 K, and the measured diffusivities are both 2% smaller than the estimated values.

**References:**

[1] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

## 2.8 $CHCl_2CHCl_2$, $CCl_3CHCl_2$, and $CH_2ClCH_2OH$

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CHCl_2CHCl_2$ | air | [1] | 298 | 760 | 55±1 | 57 | -2 |
| $CCl_3CHCl_2$ | air | [1] | 298 | 760 | 51±1 | 53 | -2 |
| $CH_2ClCH_2OH$ | air | [1] | 298 | 760 | 73±1 | 76 | -2 |

Lugg [1] measured the diffusivities of $CHCl_2CHCl_2$, $CCl_3CHCl_2$, and $CH_2ClCH_2OH$ in air at 298 K, and the measured diffusivities are all 2% smaller than the estimated values.

**References:**

[1] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

## 2.9 $CH_2$=CHCl, CHCl=CHCl, CHCl=$CCl_2$, and $CCl_2$=$CCl_2$

| formula | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CH_2$=CHCl | air | [1] | 298 | 760 | 93±4 | 85 | -2 |
| CHCl=CHCl | air | [1] | 298 | 760 | 87±7 | 71 | -2 |
| CHCl=$CCl_2$ | air | [2] | 298 | 760 | 67±1 | 63 | -2 |
| $CCl_2$=$CCl_2$ | air | [2] | 298 | 760 | 61±1 | 58 | -2 |

Barr and Watts [1] measured the diffusivities of $CH_2$=CHCl and CHCl=CHCl in air at 298 K, and Lugg [2] measured the diffusivities of CHCl=$CCl_2$ and $CCl_2$=$CCl_2$ in air at 298 K. The measured diffusivities are all 2% smaller than the estimated values.

**References:**


[1] Barr, R. F., and Watts, H.: Diffusion of some organic and inorganic compounds in air, ***J. Chem. Eng. Data***, 17, 45-46, 1972.

[2] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

# 3 Compounds with three or more carbon atoms

## 3.1 $CH_3CH_2CH_2Cl$, $CH_3CH_2CH_2Br$, and $CH_3CHBrCH_3$

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CH_3CH_2CH_2Cl$ | He | [1] | 428 | 760 | 480±7 | 474 | 1 |
| $CH_3CH_2CH_2Br$ | He | [1] | 428 | 760 | 450±7 | 475 | -5 |
| | air | [2] | 298 | 760 | 67±1 | 73 | -8 |
| $CH_3CHBrCH_3$ | He | [1] | 428 | 760 | 461±9 | 474 | -3 |
| | air | [2] | 298 | 760 | 69±1 | 73 | -4 |

The measured diffusivity of $CH_3CH_2CH_2Cl$ in He at 428 K [1] is only 1% larger than the estimated value.

The measured diffusivities of $CH_3CH_2CH_2Br$ in He at 428 K [1] and in air at 298 K [2] are 5% and 8% smaller than the estimated values, respectively.

The measured diffusivities of $CH_3CHBrCH_3$ in He at 428 K [1] and in air at 298 K [2] are 3% and 4% smaller than the estimated values, respectively.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

### 3.2 $CH_3CH_2CH_2I$ and $CH_3CHICH_3$

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CH_3CH_2CH_2I$ | He | [1] | 430 | 760 | 440±5 | 449 | -2 |
| | $H_2$ | [2] | 303 | 760 | 258 | 297 | -13 |
| | $N_2$ | [2] | 303 | 760 | 60 | 67 | -11 |
| | air | [3] | 298 | 760 | 66±1 | 63 | 5 |
| $CH_3CHICH_3$ | He | [1] | 430 | 760 | 440±9 | 449 | -2 |
| | air | [3] | 298 | 760 | 67±1 | 63 | 6 |

The measured diffusivities of $CH_3CH_2CH_2I$ in He at 430 K,[1] in $H_2$ at 303 K,[2] in $N_2$ at 303 K,[2] and in air at 298 K [3] are 2% smaller, 13% smaller, 11% smaller, and 5% larger than the estimated values.

The measured diffusivities of $CH_3CHICH_3$ in He at 430 K [1] and in air at 298 K [3] are 2% smaller and 6% larger than the estimated values.

**References:**


[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Byrne, J. J., Maguire, D., and Clarke, J. K. A.: Gas-phase interdiffusion coefficients for some polar organic compounds, ***J. Phys. Chem.***, 71, 3051-3052, 1967.

[3] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

### 3.3 $CH_3CHClCH_2Cl$, $CH_3CHBrCH2Cl$, $CH_3BrCHBrCH_2Cl$, and $CH_2=CHCH_2Cl$

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| $CH_3CHClCH_2Cl$ | air | [1] | 298 | 760 | 60±1 | 63 | -3 |
| $CH_3CHBrCH_2Cl$ | He | [2] | 427 | 760 | 433±12 | 423 | 2 |
| $CH_2BrCHBrCH_2Cl$ | air | [1] | 298 | 760 | 52±1 | 58 | -9 |
| $CH_2=CHCH_2Cl$ | air | [1] | 298 | 760 | 74±1 | 73 | 2 |

The measured diffusivities in air at 298 K [1] are 3% smaller than the estimated value for $CH_3CHCH_2Cl$, 9% smaller for $CH_3CHBrCH_2Cl$, and 2% larger for $CH_2=CHCH_2Cl$, respectively.

The measured diffusivity of $CH_3CHBrCH_2Cl$ in He at 427 K [2] is 2% larger than the estimated value.

**References:**


[1] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

[2] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

### 3.4 1-chlorobutane and 2-chlorobutane

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| 1-chlorobutane | He | [1] | 429 | 760 | 422±8 | 425 | -1 |
| | air | [2] | 296 | 744 | 67±1 | 63 | 8 |
| | | | 296 | 743 | 68 | 63 | 8 |
| | | | 295 | 748 | 67 | 62 | 7 |
| 2-chlorobutane | He | [1] | 429 | 760 | 426±6 | 425 | 0 |

The differences between the measured and estimated diffusivities in He at 429 K are around 1% for both 1-chlorobutane and 2-chlorobutane.[1]

The average measured diffusivity of 1-chlorobutane in air at 296 K [2] is 8% larger than the estimated value.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, J. Phys. Chem., 73, 3679-3685, 1969.

[2] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, Journal of Heat Transfer, 91, 259-265, 1969.

### 3.5 1–bromobutane and 2-bromobutane

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| 1-bromobutane | He | [1] | 427 | 760 | 414±5 | 421 | -2 |
| | $H_2$ | [2] | 303 | 760 | 253 | 281 | -10 |
| | $N_2$ | [2] | 303 | 760 | 61 | 68 | -10 |
| 2-bromobutane | He | [1] | 427 | 760 | 420±10 | 422 | -1 |

The measured diffusivities of 1-bromobutane in He at 427 K,[1] in $H_2$ at 303 K,[2] and in $N_2$ at 303 K [2] are 2%, 10%, and 10% smaller than the estimated values.

The difference between the measured [1] and estimated diffusivities of 2-bromobutane in He at 427 K is less than 1%.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Byrne, J. J., Maguire, D., and Clarke, J. K. A.: Gas-phase interdiffusion coefficients for some polar organic compounds, ***J. Phys. Chem.***, 71, 3051-3052, 1967.

### 3.6 1-iodobutane, 2-iodobutane, and dichloroethyl ether

| Species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| 1-iodobutane | He | [1] | 428 | 760 | 398±5 | 402 | -1 |
| 2-iodobutane | He | [1] | 427 | 760 | 414±10 | 400 | 3 |
| dichloroethyl ether | air | [2] | 298 | 760 | 53 | 55 | -5 |

The differences between the measured and estimated diffusivities are 1% for 1-iodobutane in He at 428 K,[1] 3% for 2-iodobutane in He at 427 K,[1] and 5% for dichloroethyl ether in air at 298 K,[2] respectively.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

### 3.7 1-chloropentane and 1-bromo-3-methyl-butane

| species | bath gas | reference | T | P | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| 1-chloropentane | He | [1] | 428 | 760 | 394±3 | 385 | 2 |
| 1-bromo-3-methyl-butane | $H_2$ | [2] | 303 | 760 | 235 | 258 | -9 |
| | $N_2$ | [2] | 303 | 760 | 61 | 62 | -2 |
| | Ar | [2] | 303 | 760 | 50 | 56 | -11 |

The measured diffusivity of 1-chloropentane in He at 428 K [1] is 2% larger than the estimated value.

Byrne et al.[2] measured the diffusivities of 1-bromo-3-methyl-butane at 303 K. The differences between measurements and estimations are 9%, 2%, and 11% for diffusivities in $H_2$, $N_2$, and Ar, respectively.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Byrne, J. J., Maguire, D., and Clarke, J. K. A.: Gas-phase interdiffusion coefficients for some polar organic compounds, ***J. Phys. Chem.***, 71, 3051-3052, 1967.

### 3.8 1-fluorohexane, 1-bromohexane, 2-bromohexane, and 3-bromohexane

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| 1-fluorohexane | He | [1] | 432 | 760 | 374±5 | 369 | 1 |
| 1-bromohexane | He | [1] | 428 | 760 | 350±6 | 354 | -1 |
| 2-bromohexane | He | [1] | 428 | 760 | 357±9 | 354 | 1 |
| 3-bromohexane | He | [1] | 429 | 760 | 356±33 | 355 | 1 |

Fuller et al.[1] measured the diffusivities of 1-fluorohexane, 1-bromohexane, 2-bromohexane, and 3-bromohexane in He at ~430 K. The differences between the measured and estimated diffusivities are around 1% for all the four compounds.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

### 3.9 $C_7F_{18}$

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| $C_8H_{18}$ | [1] | 303 | 760 | 9.0±0.2 | 11.0 | -18 |
| | | 323 | 760 | 10.2±0.5 | 12.3 | -17 |

The measured diffusivities of $C_7F_{18}$ in $C_8H_{18}$ [1] are 18% smaller than the estimated value at 303 K and 17% smaller at 323 K.

**References:**

[1] Weissman, S.: Estimation of diffusion coefficients from viscosity measurements-polar + polyatomic gases, ***J. Chem. Phys.***, 40, 3397-3406, 1964.

# 4 Aromatic compounds

## 4.1 fluorobenzene, chlorobenzene, and bromobenzene

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| fluorobenzene | He | [1] | 430 | 760 | 430±6 | 395 | 9 |
| | $H_2$ | [2] | 303 | 760 | 287 | 263 | 9 |
| | $N_2$ | [2] | 303 | 760 | 70 | 63 | 11 |
| | air | [3] | 295 | 734 | 61 | 58 | 4 |
| | | [3] | 295 | 729 | 61 | 58 | 5 |
| | | [3] | 295 | 735 | 61 | 58 | 4 |
| | Ar | [2] | 303 | 760 | 63 | 57 | 10 |
| chlorobenzene | He | [1] | 431 | 760 | 412±5 | 386 | 7 |
| | air | [4] | 299 | 760 | 56 | 57 | -2 |
| | | [4] | 313 | 760 | 60 | 62 | -3 |
| | | [4] | 332 | 760 | 68 | 69 | -1 |
| | | [5] | 298 | 760 | 57 | 57 | -1 |
| bromobenzene | He | [1] | 427 | 760 | 413±8 | 379 | 9 |

The diffusivity of fluorobenzene in He at 430 K was measured by Fuller et al.,[1] and the measured diffusivity is 9% larger than the estimated value.

The diffusivity of fluorobenzene in $H_2$ at 303 K was measured by Byrne et al.,[2] and the measured diffusivity is 9% larger than the estimated value.

The diffusivity of fluorobenzene in Ar at 303 K was measured by Byrne et al.,[2] and the measured diffusivity is 10% larger than the estimated value.

The diffusivity of fluorobenzene in N2 at 303 K, measured by Byrne et al.,[2] is 11% larger than the estimated value.

The average diffusivity of fluorobenzene in N2 at 295 K, measured by Grob and Elwakil,[3] is ~5% larger than the estimated value.

Fuller et al.[1] measured the diffusivity of chlorobenzene in He, and the measured diffusivity is 7% larger than the estimated value.

The diffusivities of chlorobenzene in air were measured by two studies.[4, 5] The diffusivities from 299 to 332 K, measured by Gilliland,[4] are around 3% (or less) smaller than the estimated values, and the diffusivity at 298 K, measured by Lugg,[5] is only 1% smaller than the estimated value.

The diffusivity of bromobenzene in He, measured by Fuller et al.,[1] is 9% larger than the estimated value.

**References:**


[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Byrne, J. J., Maguire, D., and Clarke, J. K. A.: Gas-phase interdiffusion coefficients for some polar organic compounds, ***J. Phys. Chem.***, 71, 3051-3052, 1967.

[3] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, Journal of Heat Transfer, 91, 259-265, 1969.

[4] Gilliland, E. R.: Diffusion coefficients in gaseous systems, ***Industrial and Engineering Chemistry***, 26, 681-685, 1934.

[5] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.

### 4.2 hexafluorobenzene

| bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|
| He | [1] | 429 | 760 | 344±6 | 314 | 10 |

The diffusivity of hexafluorobenzene in He at 429 K, measured by Fuller et al.,[1] is 10% larger than the estimated value.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

## 4.3 4-fluorotoluene, 2-chlorotoluene, 3-chlorotoluene, 4-chlorotoluene, and benzyl chloride

| species | bath gas | reference | $T$ | $P$ | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---|---|---|---|---|---|---|---|
| 4-fluorotoluene | He | [1] | 432 | 760 | 386±5 | 366 | 5 |
| 2-chlorotoluene | air | [2] | 298 | 760 | 52 | 53 | -1 |
| 3-chlorotoluene | air | [2] | 298 | 760 | 49 | 53 | -7 |
| 4-chlorotoluene | air | [2] | 298 | 760 | 47 | 53 | -11 |
| benzyl chloride | air | [2] | 298 | 760 | 54 | 53 | 2 |

The diffusivity of 4-fluorotoluene in He at 432 K, measured by Fuller et al.,[1] is 5% larger than the estimated value.

Lugg [2] measured the diffusivities of 2-chlorotoluene, 3-chlorotoluene, 4-chlorotoluene, and benzyl chloride in air at 298 K. The differences between the measured and estimated diffusivities are 1%, 7%, 11%, and 2% for 2-chlorotoluene, 3-chlorotoluene, 4-chlorotoluene, and benzyl chloride, respectively.

**References:**

[1] Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. Effect of structure on collision cross sections, ***J. Phys. Chem.***, 73, 3679-3685, 1969.

[2] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Analytical Chemistry***, 40, 1072-1077, 1968.