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 \( \text{cm}^2 \text{s}^{-1} \), and Fuller’s semi-empirical method is used in this work to estimate diffusivities \( D_e \) in the unit of Torr \( \text{cm}^2 \text{s}^{-1} \).
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1 Compounds with one carbon atom

1.1 CH₃Cl

| bath gas | reference. | T  | P  | Dm  | De  | (Dm-De)/De (%) |
|----------|------------|----|----|-----|-----|----------------|
| air      | [1]        | 298| 760| 109±2| 99  | 10             |
| CH₄      | [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              |
| SO₂      | [3]        | 303| 760| 53   | 65  | -19            |
|          |            | 313| 760| 56   | 69  | -19            |
|          |            | 323| 760| 58   | 73  | -20            |
|          |            | 333| 760| 63   | 77  | -18            |
| CH₃OCH₃  | [3]        | 303| 760| 51   | 66  | -21            |
|          |            | 313| 760| 55   | 69  | -21            |
|          |            | 323| 760| 57   | 73  | -22            |
|          |            | 333| 760| 62   | 77  | -20            |

The diffusivity of CH₃Cl 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 diffusivities of CH₃Cl in CH₄ from 298 to 438 K,[2] and the differences between the measured and estimated diffusivities are <5% across the entire temperature range.

The diffusivities of CH₃Cl in SO₂ and CH₃OCH₃, 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 modified 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, dimethyl ether and methyl chlorine, *Transactions of the Faraday Society*, 62, 3331-3337, 1966.
1.2 CH$_3$I

| 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$_3$I 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$_2$F$_2$

| 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$_2$F$_2$ in He, measured at 431 K by Fuller et al.,$^{[1]}$ is 5% 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.
1.4 CH$_2$Cl$_2$

| 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$_2$Cl$_2$ in He at 428 K, measured Fuller et al.,$^{[1]}$ is 3% larger than the estimated value.

The diffusivities of CH$_2$Cl$_2$ 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$_2$Cl$_2$ 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 CH₂ClBr

| 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 CH₂ClBr 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$_2$Br$_2$

| 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$_2$Br$_2$ 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 CHCl₃

| bath gas | reference | T     | P   | Dₘ   | Dₑ   | (Dₘ-Dₑ)/Dₑ (%) |
|----------|-----------|-------|-----|------|------|-----------------|
| He       | [1]       | 429   | 760 | 474±9 | 483  | -2              |
| N₂       | [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               |
|          |           | 298   | 760 | 67±1 | 69   | -2              |
|          |           | 323   | 760 | 83±2 | 79   | 5               |
|          |           | 298   | 760 | 66±1 | 69   | -5              |
|          | [4]       | 298   | 760 | 69   | 69   | 0               |
|          |           | 308   | 760 | 73   | 73   | 0               |
|          |           | 318   | 760 | 77   | 77   | 0               |
|          |           | 328   | 760 | 81   | 81   | 0               |
| CO₂      | [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             |
| C₂H₅OC₂H₅| [9]       | 293   | 760 | 22   | 30   | -25             |

The diffusivity of CHCl₃ 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 CHCl₃ in N₂ 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 CHCl₃ 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 CHCl₃ in CO₂ 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, and the measured diffusivities are around 13% smaller than the estimated values.

The diffusivity of CHCl$_3$ in C$_2$H$_5$OC$_2$H$_5$ at 293 K, measured by Weissman, 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 CHBr₃

| 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 CHBr₃ 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 CF₂Cl₂

| bath gas            | reference | $T$  | $P$  | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|---------------------|-----------|------|------|-------|-------|---------------------|
| air                 | [1]       | 298  | 760  | 72±3  | 67    | 7                   |
| H₂O                 | [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 CF₂Cl₂ in air,[1] H₂O,[2] ethanol,[2] and benzene [2] at 295 K and estimated values are 7%, 11%, 14%, and 4%, respectively.

Briks et al.[3] measured the diffusivities of CF₂Cl₂ 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 of 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 CF₄

| bath gas     | reference | T  | P  | $D_m$ | $D_e$ | ($D_m-D_e$)/$D_e$ (%) |
|--------------|-----------|----|----|-------|-------|-----------------------|
| CH₄          | [1]       | 298| 760| 92.7  | 87.6  | 6                     |
|              |           | 353| 760| 126.9 | 117.5 | 8                     |
|              |           | 383| 760| 145.9 | 135.5 | 8                     |
| SF₆          | [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                    |
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-hexane from 283 to 328 K, and the measured diffusivities are 11% to 15% larger than the estimated values.

Wilhelm et al. [4] measured the diffusivities of CF$_4$ in cyclohexane from 283 to 343 K, and the measured diffusivities are ~15% larger than the estimated values.

The diffusivities of CF$_4$ in benzene are measured 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 \cite{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:

\cite{1} Mueller, C. R., and Cahill, R. W.: Mass spectrometric measurement of diffusion coefficients, \textit{J. Chem. Phys.}, 40, 651-654, 1964.

\cite{2} Raw, C. J. G., and Tang, H.: Viscosity and diffusion coefficients of gaseous sulfur hexafluoride-carbon tetrafluoride mixtures, \textit{J. Chem. Phys.}, 39, 2616-2618, 1963.

\cite{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, \textit{J. Chem. Eng. Data}, 17, 187-189, 1972.

\cite{4} Wilhelm, E., Battino, R., and Carpente.RI: Binary gaseous diffusion-coefficients .2. methane and carbon tetrafluoride with cyclohexane, methylcyclohexane, benzene, and toluene at 1atm at 10-70 degrees c, \textit{J. Chem. Eng. Data}, 19, 245-246, 1974.
1.11 CCl₄

| bath gas | reference | $T$ (K) | $P$ (kPa) | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|----------|-----------|---------|---------|-------|-------|-------------------|
| N₂       | [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     | 762     | 67    | 67    | 1                 |
| CO₂      | [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                |
| CH₂Cl₂   | [10]      | 293     | 760     | 22±1  | 29    | -26               |
|          |           | 353     | 760     | 32±1  | 40    | -21               |
|          |           | 413     | 760     | 42±4  | 53    | -22               |
| CHCl₃    | [10]      | 293     | 760     | 20±1  | 24    | -17               |

The diffusivities of CCl₄ in N₂ 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$_2$Cl$_2$ 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, \textit{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, \textit{International Journal of Electronics}, 22, 381-385, 1967.
[3] Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, \textit{Analytical Chemistry}, 40, 1072-1077, 1968.
[4] Cowie, M., and Watts, H.: Diffusion of methane and chloromethanes in air, \textit{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, \textit{Aiche J.}, 13, 577-580, 1967.
[6] Grob, A. K., and Elwakil, M. M.: An interferometric technique for measuring binary diffusion coefficients, \textit{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$_2$O, CCl$_3$NO$_2$, and CNCl

| species      | bath gas | reference | $T$  | $P$  | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|--------------|----------|-----------|------|------|-------|-------|---------------------|
| CCl$_2$O     | air      | [1]       | 273  | 760  | 72    | 66    | 9                   |
| CCl$_3$NO$_2$| 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$_2$O and 1% larger for CNCl.$^{[1]}$

Two studies measured the diffusivities of CCl$_3$NO$_2$ 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 CH₃CH₂Cl

| bath gas | reference | T     | P    | \(D_m\) | \(D_e\) | \((D_m-D_e)/D_e\) (%) |
|----------|-----------|-------|------|---------|---------|------------------------|
| CH₃Cl    | [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 CH₃Cl from 298 to 438 K, and the differences between the measured and estimated diffusivities are around 22% or less.

The diffusivities of CH₃CH₂Cl in Kr were measured from 275 to 318 K by Singh and Srivastava,[2] and the differences between the measured and estimated diffusivities are smaller than 10%.

References:

[1] Gotoh, S., Manner, M., Sorensen, J. P., and Stewart, W. E.: Binary diffusion-coefficients of low-density gases I. Measurements by modified 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 CH₃CH₂Br

| bath gas | reference | T  | P  | Dₘ | Dₑ | (Dₘ-Dₑ)/Dₑ (%) |
|----------|-----------|----|----|-----|----|----------------|
| 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 CH₃CH₂Br 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] measure the diffusivities of CH₃CH₂Br 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 CH₃CH₂I

| 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 CH₃CH₂I in air at 295 K, measured by Grob and Elwakil,[1] is ~3% larger than the estimated value.

The diffusivity of CH₃CH₂I 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 \text{CH}_3\text{CHF}_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.,\textsuperscript{[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, \textit{J. Phys. Chem.}, 73, 3679-3685, 1969.
### 2.5 CH₂ClCH₂Cl

| 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 CH₂ClCH₂Cl in He at 427 K, measured by Fuller et al.,[1] is 9% larger than the estimated value.

The diffusivities of CH₂ClCH₂Cl 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 CH₂BrCH₂Br

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

The diffusivity of CH₂BrCH₂Br 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 CCl₃CH₃ and CHCl₂CH₂Cl

| species        | reference | bath gas | T  | P     | Dₘ    | Dₑ    | (Dₘ-Dₑ)/Dₑ (%) |
|---------------|-----------|----------|----|-------|-------|-------|-----------------|
| CCl₃CH₃       | [1]       | air      | 298| 760   | 60±1  | 62    | -2              |
| CHCl₂CH₂Cl    | [1]       | air      | 298| 760   | 60±1  | 62    | -2              |

Lugg [1] measured the diffusivities of CCl₃CH₃ and CHCl₂CH₂Cl 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 CHCl₂CHCl₂, CCl₃CHCl₂, and CH₂ClCH₂OH

| species            | bath gas | reference | T  | P   | \(D_m\) | \(D_e\) | \((D_m-D_e)/D_e\) (%) |
|--------------------|----------|-----------|----|-----|---------|---------|-----------------------|
| CHCl₂CHCl₂         | air      | [1]       | 298| 760 | 55±1    | 57      | -2                    |
| CCl₃CHCl₂          | air      | [1]       | 298| 760 | 51±1    | 53      | -2                    |
| CH₂ClCH₂OH         | air      | [1]       | 298| 760 | 73±1    | 76      | -2                    |

Lugg\(^{[1]}\) measured the diffusivities of CHCl₂CHCl₂, CCl₃CHCl₂, and CH₂ClCH₂OH 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.
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 CH₃CH₂CH₂Cl, CH₃CH₂CH₂Br, and CH₃CHBrCH₃

| species          | bath gas | reference | $T$  | $P$  | $D_m$   | $D_e$ | ($D_m - D_e$)/$D_e$ (%) |
|------------------|----------|-----------|------|------|---------|-------|-------------------------|
| CH₃CH₂CH₂Cl      | He       | [1]       | 428  | 760  | 480±7   | 474   | 1                       |
| CH₃CH₂CH₂Br      | He       | [1]       | 428  | 760  | 450±7   | 475   | -5                      |
|                  | air      | [2]       | 298  | 760  | 67±1    | 73    | -8                      |
| CH₃CHBrCH₃       | He       | [1]       | 428  | 760  | 461±9   | 474   | -3                      |
|                  | air      | [2]       | 298  | 760  | 69±1    | 73    | -4                      |

The measured diffusivity of CH₃CH₂CH₂Cl in He at 428 K [1] is only 1% larger than the estimated value.

The measured diffusivities of CH₃CH₂CH₂Br 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 CH₃CHBrCH₃ 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 CH₃CH₂CH₂I and CH₃CHICH₃

| species        | bath gas | reference | T   | P   | Dₘ  | Dₑ  | (Dₘ-Dₑ)/Dₑ (%) |
|----------------|----------|-----------|-----|-----|-----|-----|-----------------|
| CH₃CH₂CH₂I     | He       | [1]       | 430 | 760 | 440±5 | 449 | -2              |
|                | H₂       | [2]       | 303 | 760 | 258  | 297 | -13             |
|                | N₂       | [2]       | 303 | 760 | 60   | 67  | -11             |
|                | air      | [3]       | 298 | 760 | 66±1 | 63  | 5               |
| CH₃CHICH₃      | He       | [1]       | 430 | 760 | 440±9 | 449 | -2              |
|                | air      | [3]       | 298 | 760 | 67±1 | 63  | 6               |

The measured diffusivities of CH₃CH₂CH₂I in He at 430 K,[1] in H₂ at 303 K,[2] in N₂ 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 CH₃CHICH₃ 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 CH₃CHClCH₂Cl, CH₃CHBrCH₂Cl, CH₃BrCHBrCH₂Cl, and CH₂=CHCH₂Cl

| species            | bath gas | reference | T    | P    | $D_m$ | $D_e$ | $(D_m-D_e)/D_e$ (%) |
|--------------------|----------|-----------|------|------|-------|-------|---------------------|
| CH₃CHClCH₂Cl       | air      | [1]       | 298  | 760  | 60±1  | 63    | -3                  |
| CH₃CHBrCH₂Cl       | He       | [2]       | 427  | 760  | 433±12| 423   | 2                   |
| CH₂BrCHBrCH₂Cl     | air      | [1]       | 298  | 760  | 52±1  | 58    | -9                  |
| CH₂=CHCH₂Cl        | 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 CH₃CHCH₂Cl, 9% smaller for CH₃CHBrCH₂Cl, and 2% larger for CH₂=CHCH₂Cl, respectively.

The measured diffusivity of CH₃CHBrCH₂Cl 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              |          |           | 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.
The measured diffusivities of $\text{C}_7\text{F}_{18}$ in $\text{C}_8\text{H}_{18}$\textsuperscript{[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 | $T$   | $P$   | $D_m$  | $D_c$  | $(D_m-D_c)/D_c$ (%) |
|---------------|----------|-----------|-------|-------|--------|--------|---------------------|
| 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 N$_2$ at 303 K, measured by Byrne et al.,[2] is 11% larger than the estimated value.

The average diffusivity of fluorobenzene in N$_2$ 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.,\textsuperscript{[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, \textit{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    | $D_m$  | $D_c$  | $(D_m-D_c)/D_c$ (%) |
|------------------|----------|-----------|------|------|--------|--------|-------------------|
| 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.