Diffusion coefficient for gases

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1 Binary diffusion coefficient of nonpolar gases

The binary diffusion coefficient between two nonpolar gases A and B are given Wilke and Lee is as follows:

$$D_{AB} = \frac{[3.03 - \frac{0.98}{\sqrt{M_{AB}}}] \times 10^{-3} T^{\frac{3}{2}}}{P\sqrt{M_{AB}}\sigma_{AB}^2 \Omega_D}$$

where

D_{AB} = binary diffusion coefficient, cm^2/s
T = temperature, K
M_A, M_B = molecular weights of A and B, g/mol
M_{AB} = $2\frac{1}{\frac{1}{M_A}+\frac{1}{M_B}}$
P = pressure, bar

$\sigma_{AB} = \frac{\sigma_a + \sigma_B}{2}$, where $\sigma_A = 1.18 V_{b_A}^{\frac{1}{3}}$ and $\sigma_B = 1.18 V_{b_B}^{\frac{1}{3}}$. V_{b_A} is the liquid molar volume ($\mathrm{cm}^3/\mathrm{mol}$).

$$\Omega_D = \frac{A}{T^{*B}} + \frac{C}{e^{DT*}} + \frac{E}{e^{FT*}} + \frac{G}{e^{HT*}}$$

$$T^* = \frac{kT}{\epsilon_{AB}}, A = 1.06036, B = 0.15610$$
$$C = 0.19300, D = 0.47635, E = 1.03587$$
$$F = 1.52996, G = 1.76474, H = 3.89411$$

$$(\frac{\epsilon}{k})_A = 1.15T_{b_A}$$
$$(\frac{\epsilon}{k})_B = 1.15T_{b_B}$$
$$\epsilon_{AB} = \sqrt{(\frac{\epsilon}{k})_A(\frac{\epsilon}{k})_B}$$

T_b is the normal boiling temperature at 1 atmosphere pressure in Kelvin.