SUPPLEMENTARY INFORMATION

Liu's equation:[79]

$$D = \frac{\kappa}{\beta^2 \rho} exp\left(\frac{-0.75\beta^3\rho}{1.2588 - \beta^3\rho} - \gamma\right)$$

At constant temperature, the previous equation relates a bulk fluid self-diffusion coefficient, D, with the corresponding number density, ρ, using three numeric constants characteristic of each substance, namely κ, β, and γ, according to:

$$\kappa = 21.16\sqrt{1000\,RT/M}$$

$$\beta = \sigma_{LJ} 2^{1/6}\left[1 + \sqrt{\frac{1.3229T}{\varepsilon_{LJ}/k_B}}\right]^{-1/6}$$

$$\gamma = -\frac{0.27862\left(\varepsilon_{LJ}/k_B\right)}{T}$$

where, k_B is the Boltzmann constant (1.38065×10^{-23} J·K^{-1}), R is the ideal gas constant (8.314472 J·K^{-1}mol^{-1}) and M is the molecular mass. Thus, to obtain the complete (ρ, T) surface, the only inputs are the Lennard-Jones potential parameters of the fluid (σ_{LJ}, ε_{LJ}).