

Standard deviation :

$$y_{\text{sim}} = y_1 + \frac{(T_{\text{exp}} - T_1)(y_2 - y_1)}{T_2 - T_1}$$

$$\text{Absolute error} = y_{\text{sim}} - y_{\text{exp}}$$

$$\bar{\epsilon} = \frac{1}{N} \sum_{i=1}^N \epsilon_i$$

$$\text{Variance} = \frac{1}{N-1} \sum_{i=1}^N (\epsilon_i - \bar{\epsilon})^2$$

$$\text{Standard deviation} = \sqrt{\text{Variance}}$$

- T_{exp} : Experimental temperature point.
- T_1, T_2 : Nearest simulated temperature points bracketing T_{exp} .
- y_1, y_2 : Simulated values at T_1 and T_2 .
- y_{sim} : Interpolated simulated value at T_{exp} .
- y_{exp} : Experimental value.
- y_{sim} : Interpolated simulated value
- ϵ_i : Absolute error for the i -th data point.
- N : Number of data points.

S-table.1 The absolute error calculated from simulated data, referenced against experimental data.

Temperature	Self-diffusion coefficients (experimental value cm ² /s)	Self-diffusion coefficients (interpolated simulated value cm ² /s)	Absolute error
1100K	6.35×10 ⁻⁵	9.62×10 ⁻⁵	3.27×10 ⁻⁵
1110K	6.54×10 ⁻⁵	1.02×10 ⁻⁴	3.68×10 ⁻⁵
1120K	6.74×10 ⁻⁵	1.08×10 ⁻⁴	4.08×10 ⁻⁵
1140K	7.15×10 ⁻⁵	1.20×10 ⁻⁴	4.87×10 ⁻⁵
1160K	7.57×10 ⁻⁵	1.32×10 ⁻⁴	5.65×10 ⁻⁵
1180K	7.99×10 ⁻⁵	1.22×10 ⁻⁴	4.17×10 ⁻⁵
1200K	8.42×10 ⁻⁵	1.38×10 ⁻⁴	5.34×10 ⁻⁵
1220K	8.86×10 ⁻⁵	1.54×10 ⁻⁴	6.50×10 ⁻⁵
1260K	9.32×10 ⁻⁵	1.39×10 ⁻⁴	4.61×10 ⁻⁵
1280K	9.77×10 ⁻⁵	1.57×10 ⁻⁴	5.96×10 ⁻⁵
1300K	1.02×10 ⁻⁴	1.41×10 ⁻⁴	3.94×10 ⁻⁵
1300K	1.07×10 ⁻⁴	1.65×10 ⁻⁴	5.84×10 ⁻⁵
1310K	1.09×10 ⁻⁴	1.77×10 ⁻⁴	6.84×10 ⁻⁵

The standard deviation of the absolute error between the simulated values and the experimental values is 9.58×10⁻⁶