

1-Chloro-1-nitropropane
600-25-9 | DTXSID2024797

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 8.93×10^{-13} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.32×10^{-1}

Confidence level: 6.86×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Nitric acid, 1-methylethyl ester

Measured: 4.90×10^{-13}

Predicted: 7.48×10^{-13}

Image not found

n-Propyl nitrate

Measured: 7.30×10^{-13}

Predicted: 8.54×10^{-13}

Image not found

Dimethylnitramine

Measured: 3.84×10^{-12}

Predicted: 1.45×10^{-12}

Image not found

1-Nitropropane

Measured: 4.40×10^{-13}

Predicted: 5.94×10^{-13}

Image not found

Butyl nitrate

Measured: 1.71×10^{-12}

Predicted: 1.60×10^{-12}