

Isopropyl ether
108-20-3 | DTXSID4021890

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: 9.87×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.99×10^{-1}

Confidence level: 7.68×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Isopropyl ether

Measured: 1.02×10^{-11}

Predicted: 9.87×10^{-12}

Image not found

2-Methyl-2-ethoxypropane

Measured: 8.84×10^{-12}

Predicted: 7.89×10^{-12}

Image not found

2-Methyltetrahydrofuran

Measured: 2.20×10^{-11}

Predicted: 1.69×10^{-11}

Image not found

Butane, 1-methoxy-

Measured: 1.48×10^{-11}

Predicted: 1.70×10^{-11}

Image not found

Methyl tert-butyl ether

Measured: 2.94×10^{-12}

Predicted: 6.19×10^{-12}