

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.68e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.81e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

Image not found

Propane, 1-(1-methylethoxy)-

Measured: 4.60e-02

Predicted: 6.37e-02

Image not found

2-Methyl-2-ethoxypropane

Measured: 1.17e-01

Predicted: 5.28e-02

Image not found

Propyl ether

Measured: 4.80e-02

Predicted: 5.81e-02

Image not found

Vinyl isobutyl ether

Measured: 3.00e-02

Predicted: 5.20e-02

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Butane, 2-ethoxy-2-methyl-

Measured: 3.44e-03

Predicted: 8.50e-03