

Butyl ether
142-96-1 | DTXSID1022007

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: 3.04e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.63e-01

Confidence level: 6.07e-01

Nearest Neighbors from the Training Set

Image not found

Butyl ether

Measured: 2.30e-03

Predicted: 3.04e-03

Image not found

2-Ethylhexylamine

Measured: 1.93e-02

Predicted: 1.01e-02

Image not found

1-Octanamine

Measured: 1.55e-03

Predicted: 4.20e-03

Image not found

Butane, 2-ethoxy-2-methyl-

Measured: 3.44e-03

Predicted: 8.50e-03

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tert-Butyl isopropyl ether

Measured: 4.30e-03

Predicted: 8.44e-03