

Isoamyl ether
544-01-4 | DTXSID8052198

Model Performance

Model	Data
-------	------

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: 1.80e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 6.34e-01

Nearest Neighbors from the Training Set

Image not found

Isoamyl ether

Measured: 1.26e-03

Predicted: 1.80e-03

Image not found

1-Decanamine

Measured: 3.50e-03

Predicted: 2.79e-03

Image not found

Butyl ether

Measured: 2.30e-03

Predicted: 3.04e-03

Image not found

Ethylene glycol dibutyl ether

Measured: 1.15e-02

Predicted: 6.65e-03

Image not found

1-Octanamine

Measured: 1.55e-03

Predicted: 4.20e-03