

Diethyl ether
60-29-7 | DTXSID3021720

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: 4.74e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.31e-01

Confidence level: 8.37e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl ether

Measured: 8.15e-01

Predicted: 4.74e-01

Image not found

Propane, 1-methoxy-

Measured: 4.11e-01

Predicted: 5.06e-01

Image not found

Ether, isopropyl methyl

Measured: 8.77e-01

Predicted: 9.40e-01

Image not found

Ether, isobutyl methyl

Measured: 1.26e-01

Predicted: 1.50e-01

Image not found

Propane, 1-ethoxy-

Measured: 1.73e-01

Predicted: 1.57e-01