

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 423 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.17e-01

Confidence level: 8.77e-01

Nearest Neighbors from the Training Set

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2-Mercaptoethanol

Measured: 538

Predicted: 7.89e-01

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Propyl isovalerate

Measured: 465

Predicted: 3.10

[Image not found](#)

Bromoacetone

Measured: 605

Predicted: 38.1

[Image not found](#)

1-Propoxy-2-propanol

Measured: 250

Predicted: 2.02

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Butane, 1-(methylthio)-

Measured: 181

Predicted: 17.9