

Diethyl sulfate
64-67-5 | DTXSID1024045

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: 1.08e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.28e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

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Diethyl sulfate

Measured: 4.54e-02

Predicted: 1.08e-01

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Trimethyl phosphate

Measured: 3.57

Predicted: 3.64

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Ethyl dimethyl phosphate

Measured: 3.24

Predicted: 3.42

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Dimethyl propyl phosphate

Measured: 2.97

Predicted: 2.43

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Methyl benzenesulphonate

Measured: 1.81e-02

Predicted: 1.15e-01