

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.95e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

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Amitrole

Measured: 2.12e-01

Predicted: 6.44e-07

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2,2-Dimethoxypropane

Measured: 6.77e-01

Predicted: 72.6

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Methoprotrolyne

Measured: 4.52

Predicted: 6.52e-07

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Cyclohexane, (1-methylethyl)-

Measured: 9.62e-01

Predicted: 4.19

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Methyl butyrate

Measured: 1.18e-02

Predicted: 32.4