

Ethane, methoxy-d3
16995-14-5 | DTXSID20168777

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: 1070 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.34e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

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1,2-Dichloroethylene

Measured: 1490

Predicted: 120

Image not found

Bromoacetone

Measured: 605

Predicted: 38.1

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2-Mercaptoethanol

Measured: 538

Predicted: 7.89e-01

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Propyl isovalerate

Measured: 465

Predicted: 3.10

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1-Tetradecanol

Measured: 4450

Predicted: 1.08e-04