

Propane, 1,1,3,3-tetramethoxy-
102-52-3 | DTXSID4059255

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: 1.78 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.33e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

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1-Bromodecane

Measured: 4.03e-02

Predicted: 2.76e-02

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Propham

Measured: 3.86

Predicted: 1.30e-04

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Propanoic anhydride

Measured: 11.0

Predicted: 9.92e-01

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Bis(2-chloroethoxy)methane

Measured: 2.96

Predicted: 1.91e-01

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Pyridine

Measured: 17.5

Predicted: 29.1