

Isopropyl ether
108-20-3 | DTXSID4021890

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: 124 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.76e-01

Confidence level: 8.66e-01

Nearest Neighbors from the Training Set

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4-Methyl-2-pentanol

Measured: 149

Predicted: 4.34

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Propanoic acid, 1-methylethyl ester

Measured: 124

Predicted: 19.4

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1-Ethyl-2,3-dimethylbenzene

Measured: 75.2

Predicted: 9.55e-01

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Butane, 1-(methylthio)-

Measured: 181

Predicted: 17.9

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1-Nitrobutane

Measured: 139

Predicted: 6.23