

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 77.0 °C

Global applicability domain: Inside

Local applicability domain index: 9.73e-01

Confidence level: 8.68e-01

Nearest Neighbors from the Training Set

Image not found

Isopropyl ether

Measured: 68.5

Predicted: 77.0

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2-Methyl-2-ethoxypropane

Measured: 73.1

Predicted: 77.9

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tert-Amyl methyl ether

Measured: 86.3

Predicted: 77.9

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Propane, 1-(1-methylethoxy)-

Measured: 83.0

Predicted: 85.2