

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -99.1 °C

Global applicability domain: Inside

Local applicability domain index: 9.01e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

Image not found

Isopropyl ether

Measured: -86.8

Predicted: -99.1

Image not found

2-Methyl-2-ethoxypropane

Measured: -94.0

Predicted: -97.3

Image not found

tert-Butyl isopropyl ether

Measured: -88.0

Predicted: -91.9

Image not found

1-Ethoxybutane

Measured: -124

Predicted: -118

Image not found

Propyl ether

Measured: -122

Predicted: -118