

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.60

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 6.13e-01

Nearest Neighbors from the Training Set

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Isopropyl ether

Measured: 1.52

Predicted: 1.60

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Methyl tert-butyl ether

Measured: 0.94

Predicted: 1.17

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2-(Hexyloxy)ethanol

Measured: 1.86

Predicted: 1.74

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Pentane

Measured: 3.39

Predicted: 3.15