

Isopentyl alcohol
123-51-3 | DTXSID3025469

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: -96.2 °C

Global applicability domain: Inside

Local applicability domain index: 8.77e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

Image not found

Isopentyl alcohol

Measured: -117

Predicted: -96.2

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1-Pentanol

Measured: -78.9

Predicted: -87.1

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1-Hexanol

Measured: -44.6

Predicted: -61.5

Image not found

2-Methyl-1-propanol

Measured: -108

Predicted: -103

Image not found

2-Butanol

Measured: -115

Predicted: -70.5