

n-Hexane
110-54-3 | DTXSID0021917

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: 62.9 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 9.01e-01

Nearest Neighbors from the Training Set

[Image not found](#)

n-Hexane

Measured: 68.7

Predicted: 62.9

[Image not found](#)

2-Methylpentane

Measured: 60.2

Predicted: 60.5

[Image not found](#)

3-Methylpentane

Measured: 63.2

Predicted: 60.5

[Image not found](#)

2,2-Dimethylbutane

Measured: 49.7

Predicted: 57.2

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2,3-Dimethylbutane

Measured: 57.9

Predicted: 57.7