

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -116 °C

Global applicability domain: Inside

Local applicability domain index: 9.46e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

[Image not found](#)

n-Hexane

Measured: -95.3

Predicted: -116

[Image not found](#)

Heptane

Measured: -90.6

Predicted: -94.2

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3-Methylpentane

Measured: -163

Predicted: -127

[Image not found](#)

Pentane

Measured: -130

Predicted: -136

[Image not found](#)

3-Methylhexane

Measured: -119

Predicted: -114