

2-Methylheptane
592-27-8 | DTXSID2060460

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: -110 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 7.90e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Methylheptane

Measured: -121

Predicted: -110

[Image not found](#)

2-Methylheptane

Measured: -109

Predicted: -110

[Image not found](#)

3-Methyloctane

Measured: -108

Predicted: -101

[Image not found](#)

4-Methyloctane

Measured: -113

Predicted: -101