

Heptane
142-82-5 | DTXSID6024127

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: 93.7 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 9.04e-01

Nearest Neighbors from the Training Set

Image not found

Heptane

Measured: 98.5

Predicted: 93.7

Image not found

3-Methylhexane

Measured: 91.0

Predicted: 89.5

Image not found

2-Methylhexane

Measured: 90.0

Predicted: 89.5

Image not found

Pentane, 3-ethyl-

Measured: 93.5

Predicted: 89.5

Image not found

Pentane,3,3-dimethyl-

Measured: 86.0

Predicted: 84.5