

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
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** -94.2 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 9.58e-01

**Confidence level:** 7.52e-01

## Nearest Neighbors from the Training Set

Image not found

Heptane

**Measured:** -90.6

**Predicted:** -94.2

Image not found

Octane

**Measured:** -56.8

**Predicted:** -68.5

Image not found

n-Hexane

**Measured:** -95.3

**Predicted:** -116

Image not found

3-Methylhexane

**Measured:** -119

**Predicted:** -114

Image not found

2-Methylhexane

**Measured:** -118

**Predicted:** -114