

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.90e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.32e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Heptane

Measured: 3.39e-05

Predicted: 3.90e-05

[Image not found](#)

3-Methylhexane

Measured: 4.94e-05

Predicted: 4.20e-05

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2-Methylhexane

Measured: 2.53e-05

Predicted: 4.32e-05

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2,4-Dimethylpentane

Measured: 5.49e-05

Predicted: 4.61e-05