

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.67

Global applicability domain: Inside

Local applicability domain index: 9.89e-01

Confidence level: 4.81e-01

Nearest Neighbors from the Training Set

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Heptane

Measured: 2.95

Predicted: 3.67

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Cyclopentanone

Measured: 3.67

Predicted: 3.70

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Trichloroethylene

Measured: 2.99

Predicted: 3.69

[Image not found](#)

N,N-Dimethylacetamide

Measured: 5.33

Predicted: 3.72

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Ethyl butyrate

Measured: 3.56

Predicted: 3.66