

n-Hexane
110-54-3 | DTXSID0021917

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: 3.19

Global applicability domain: Inside

Local applicability domain index: 9.92e-01

Confidence level: 5.38e-01

Nearest Neighbors from the Training Set

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n-Hexane

Measured: 2.40

Predicted: 3.19

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1,2-Dichloropropane

Measured: 2.96

Predicted: 3.29

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N,N-Dimethylformamide

Measured: 4.38

Predicted: 3.13

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Dibromomethane

Measured: 3.07

Predicted: 3.12

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1,4-Dioxane

Measured: 3.18

Predicted: 3.27