

Cyclohexane
110-82-7 | DTXSID4021923

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: 3.05 °C

Global applicability domain: Inside

Local applicability domain index: 9.46e-01

Confidence level: 4.18e-01

Nearest Neighbors from the Training Set

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Cyclohexane

Measured: 6.60

Predicted: 3.05

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Cyclohexane, tridecyl-

Measured: 18.5

Predicted: -66.9

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Heptadecylcyclohexane

Measured: 38.0

Predicted: -66.3

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Nonadecylcyclohexane

Measured: 45.0

Predicted: 3.82

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Propylcyclohexane

Measured: -94.9

Predicted: -66.9