

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 73.1 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 9.09e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cyclohexane

Measured: 80.7

Predicted: 73.1

[Image not found](#)

Methylcyclopentane

Measured: 71.8

Predicted: 70.1

[Image not found](#)

Cyclopropane, propyl-

Measured: 69.1

Predicted: 70.1

[Image not found](#)

Cyclobutane, ethyl-

Measured: 70.8

Predicted: 70.1