

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.22

Global applicability domain: Inside

Local applicability domain index: 9.98e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexane

Measured: 2.74

Predicted: 3.22

Image not found

Propyl ether

Measured: 2.97

Predicted: 3.22

Image not found

Isobutyl acetate

Measured: 3.45

Predicted: 3.22

Image not found

Chlorodibromomethane

Measured: 3.59

Predicted: 3.23

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1,1,2-Trichloroethane

Measured: 3.40

Predicted: 3.23