

Cyclopentane
287-92-3 | DTXSID6024886

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: 44.0 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

Image not found

Cyclopentane

Measured: 49.3

Predicted: 44.0

Image not found

Cyclobutane, methyl-

Measured: 36.3

Predicted: 35.2

Image not found

Cyclopropane, ethyl-

Measured: 35.9

Predicted: 35.2

Image not found

3-Chloro-2-methylpropene

Measured: 71.5

Predicted: 68.4

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1,1-Dimethylcyclopropane

Measured: 20.6

Predicted: 30.2