

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 24.0

Global applicability domain: Inside

Local applicability domain index: 5.19e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

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Cyclohexane

Measured: 83.2

Predicted: 59.1

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Quinoline

Measured: 3.80

Predicted: 6.66

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Benzene

Measured: 4.27

Predicted: 10.0

[Image not found](#)

Methylcyclohexane

Measured: 186

Predicted: 233

[Image not found](#)

N-Methylaniline

Measured: 10.0

Predicted: 5.88