

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 7.04×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.38×10^{-1}

Confidence level: 8.02×10^{-1}

Nearest Neighbors from the Training Set

[Image not found](#)

Cyclohexane

Measured: 7.49×10^{-12}

Predicted: 7.04×10^{-12}

[Image not found](#)

Cycloheptane

Measured: 1.25×10^{-11}

Predicted: 9.38×10^{-12}

[Image not found](#)

Cyclopentane

Measured: 5.16×10^{-12}

Predicted: 6.13×10^{-12}

[Image not found](#)

Cyclooctane

Measured: 1.37×10^{-11}

Predicted: 9.99×10^{-12}

[Image not found](#)

Cyclobutane

Measured: 1.50×10^{-12}

Predicted: 1.78×10^{-12}