

1,3,5-Cycloheptatriene
544-25-2 | DTXSID5073909

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 27.9 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.68e-01

Confidence level: 4.76e-01

Nearest Neighbors from the Training Set

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Ethane, isothiocyanato-

Measured: 23.5

Predicted: 7.93

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1-Pentanol

Measured: 94.8

Predicted: 3.00

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1,4-Pentadiene

Measured: 97.3

Predicted: 543

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1-Pentyne

Measured: 66.6

Predicted: 435

[Image not found](#)

Decamethylcyclopentasiloxane

Measured: 5.80e-01

Predicted: 1.65e-01