

3-Methylhexane
589-34-4 | DTXSID3044334

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: 55.0 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.98e-01

Confidence level: 8.65e-01

Nearest Neighbors from the Training Set

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4-Ethylaniline

Measured: 61.5

Predicted: 6.90e-02

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1-Nitropropane

Measured: 79.4

Predicted: 9.95

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Toluene-2,4-diisocyanate

Measured: 23.4

Predicted: 6.38e-03

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Cyclohexene, 1-methyl-

Measured: 66.0

Predicted: 29.8

Image not found

Cyclohexene, 1-methyl-

Measured: 66.0

Predicted: 29.8