

2-Methylhexane
591-76-4 | DTXSID5052256

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: 58.3 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.00e-01

Confidence level: 9.09e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cyclohexene, 1-methyl-

Measured: 66.0

Predicted: 29.8

[Image not found](#)

Cyclohexene, 1-methyl-

Measured: 66.0

Predicted: 29.8

[Image not found](#)

3-Methyl-2-butanone

Measured: 68.9

Predicted: 51.5

[Image not found](#)

1-Nitropropane

Measured: 79.4

Predicted: 9.95

[Image not found](#)

4-Ethylaniline

Measured: 61.5

Predicted: 6.90e-02

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Toluene-2,4-diisocyanate

Measured: 23.4

Predicted: 6.38e-03