

2-Methylheptane
592-27-8 | DTXSID2060460

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: 14.9 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.96e-01

Confidence level: 8.98e-01

Nearest Neighbors from the Training Set

Image not found

Toluene-2,4-diisocyanate

Measured: 23.4

Predicted: 6.38e-03

Image not found

Pentane, 3-ethyl-3-methyl-

Measured: 10.1

Predicted: 29.5

Image not found

Butane, 2-ethoxy-2-methyl-

Measured: 9.02

Predicted: 55.1

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2,3,3-Trimethylhexane

Measured: 11.3

Predicted: 11.4