

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.33

Global applicability domain: Inside

Local applicability domain index: 9.88e-01

Confidence level: 7.24e-01

Nearest Neighbors from the Training Set

Image not found

Valeronitrile

Measured: 3.60

Predicted: 3.33

Image not found

Cyclohexene

Measured: 2.83

Predicted: 3.23

Image not found

1,1,2-Trichloroethane

Measured: 3.40

Predicted: 3.23

Image not found

Tetrahydropyran

Measured: 3.22

Predicted: 3.13

Image not found

Chlorodibromomethane

Measured: 3.59

Predicted: 3.23