

2,2,3-Trimethylbutane
464-06-2 | DTXSID7060047

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.60

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

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2,2-Dimethylbutane

Measured: 3.82

Predicted: 3.53

[Image not found](#)

Menthol

Measured: 3.40

Predicted: 3.31

[Image not found](#)

Di-tert-butyl ketone

Measured: 3.00

Predicted: 3.20

[Image not found](#)

4-tert-Butylcyclohexanol

Measured: 3.23

Predicted: 3.22

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2,4,4-Trimethyl-1-pentene

Measured: 4.55

Predicted: 4.33