

2,3,4-Trimethylpentane
565-75-3 | DTXSID6060343

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 13.9 days

Global applicability domain: Inside

Local applicability domain index: 6.00e-01

Confidence level: 7.54e-01

Nearest Neighbors from the Training Set

Image not found

2,3,4-Trimethylpentane

Measured: 511

Predicted: 13.9

Image not found

2,2,3-Trimethylbutane

Measured: 61.9

Predicted: 10.7

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2,4-Dimethylpentane

Measured: 7430

Predicted: 33.1

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2,2,4-Trimethylpentane

Measured: 4890

Predicted: 30.5

Image not found

2,2-Dimethylbutane

Measured: 880

Predicted: 16.2