

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 6.83 days

Global applicability domain: Inside

Local applicability domain index: 8.98e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

[Image not found](#)

3-Methylhexane

Measured: 157

Predicted: 6.83

[Image not found](#)

2-Methylhexane

Measured: 12.5

Predicted: 5.54

[Image not found](#)

3-Ethylhexane

Measured: 24.3

Predicted: 7.04