

Ethane
74-84-0 | DTXSID6026377

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: 16.5 days

Global applicability domain: Outside

Local applicability domain index: 2.83e-01

Confidence level: 8.91e-01

Nearest Neighbors from the Training Set

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Tetradecane

Measured: 1370

Predicted: 18.3

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Pentadecane

Measured: 1810

Predicted: 20.8

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Tridecane

Measured: 305

Predicted: 13.5

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Hexadecane

Measured: 681

Predicted: 20.1

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Dodecane

Measured: 201

Predicted: 10.6