

Ethyl heptanoate
106-30-9 | DTXSID1040112

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.08e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.66e-01

Confidence level: 6.76e-01

Nearest Neighbors from the Training Set

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Ethyl heptanoate

Measured: 1.83e-03

Predicted: 1.08e-03

Image not found

Methyl octanoate

Measured: 4.07e-04

Predicted: 6.30e-04

Image not found

Hexyl acetate

Measured: 3.54e-03

Predicted: 6.89e-03

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Di-tert-butyl peroxide

Measured: 6.84e-04

Predicted: 1.96e-03

Image not found

Ethyl octanoate

Measured: 4.07e-04

Predicted: 2.98e-04