

Ethyl hexanoate
123-66-0 | DTXSID3021980

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 10.1

Global applicability domain: Inside

Local applicability domain index: 5.80e-01

Confidence level: 6.28e-01

Nearest Neighbors from the Training Set

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Acetamide, N-methyl-N-phenyl-

Measured: 1.51

Predicted: 2.53

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Molinate

Measured: 25.7

Predicted: 14.8

Image not found

Butyl ether

Measured: 72.4

Predicted: 32.3

Image not found

Quinoline

Measured: 3.80

Predicted: 6.66

Image not found

N-Ethylaniline

Measured: 12.9

Predicted: 5.70