

Ethanol
64-17-5 | DTXSID9020584

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: 16.5 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.40e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

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Ethanol

Measured: 21.7

Predicted: 16.5

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Allyl alcohol

Measured: 17.2

Predicted: 14.2

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1-Propanol

Measured: 16.6

Predicted: 13.1

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Propargyl alcohol

Measured: 17.8

Predicted: 15.2

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Methallyl alcohol

Measured: 2.69

Predicted: 6.51