

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 80.5 °C

Global applicability domain: Inside

Local applicability domain index: 5.67e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

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Ethanol

Measured: 78.2

Predicted: 80.5

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Isopropanol

Measured: 82.3

Predicted: 90.0

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1-Propanol

Measured: 97.2

Predicted: 96.5

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Ethyl hydroperoxide

Measured: 95.0

Predicted: 99.9

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Methanol

Measured: 64.7

Predicted: 69.1