

Triethanolamine
102-71-6 | DTXSID9021392

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 24.5 °C

Global applicability domain: Inside

Local applicability domain index: 4.03e-01

Confidence level: 5.27e-01

Nearest Neighbors from the Training Set

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Triethanolamine

Measured: 20.5

Predicted: 24.5

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Triisopropanolamine

Measured: 45.0

Predicted: 38.8

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Diethanolamine

Measured: 28.0

Predicted: 32.8

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N-Methyldiethanolamine

Measured: -21.0

Predicted: -19.8

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1,3-Propanediol, 2-amino-2-methyl-

Measured: 110

Predicted: 84.6