

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 326 °C

Global applicability domain: Outside

Local applicability domain index: 2.88e-01

Confidence level: 4.99e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Triethanolamine

Measured: 335

Predicted: 326

[Image not found](#)

Triisopropanolamine

Measured: 305

Predicted: 302

[Image not found](#)

Diisopropanolamine

Measured: 250

Predicted: 248

[Image not found](#)

2-(Hydroxymethyl)-2-methyl-1,3-propanediol

Measured: 283

Predicted: 289

[Image not found](#)

Metaraminol

Measured: 218

Predicted: 257