

Triethylenetetramine
112-24-3 | DTXSID9023702

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: 265 °C

Global applicability domain: Outside

Local applicability domain index: 2.34e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

Image not found

Triethylenetetramine

Measured: 267

Predicted: 265

Image not found

Tetraethylenepentamine

Measured: 342

Predicted: 339

Image not found

Diethylenetriamine

Measured: 207

Predicted: 206

Image not found

1-(2-Aminoethyl)piperazine

Measured: 220

Predicted: 217

Image not found

N-(3-Aminopropyl)-N-methylpropane-1,3-diamine

Measured: 233

Predicted: 228