

2,3,4-Trinitrotoluene
602-29-9 | DTXSID60208944

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: 309 °C

Global applicability domain: Outside

Local applicability domain index: 7.12e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

Image not found

2,3,4-Trinitrotoluene

Measured: 301

Predicted: 309

Image not found

2,4,5-Trinitrotoluene

Measured: 300

Predicted: 309

Image not found

1,3,5-Trinitrobenzene

Measured: 315

Predicted: 304

Image not found

2,4-Dinitroaniline

Measured: 334

Predicted: 330

Image not found

4-Aminoazobenzene

Measured: 366

Predicted: 337