

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 113 °C

Global applicability domain: Inside

Local applicability domain index: 8.52e-01

Confidence level: 5.39e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2,3,4-Trinitrotoluene

Measured: 112

Predicted: 113

[Image not found](#)

2,4,5-Trinitrotoluene

Measured: 104

Predicted: 109

[Image not found](#)

2,4,6-Trinitrotoluene

Measured: 80.1

Predicted: 105

[Image not found](#)

2,4,6-Trinitro-m-xylene

Measured: 184

Predicted: 147

[Image not found](#)

1,3,5-Trinitrobenzene

Measured: 122

Predicted: 111