

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.94

Global applicability domain: Inside

Local applicability domain index: 5.30e-01

Confidence level: 7.71e-01

Nearest Neighbors from the Training Set

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2,6-Dinitroaniline

Measured: 1.79

Predicted: 1.64

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2,4,6-Trinitrotoluene

Measured: 1.60

Predicted: 1.66

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2,6-Dinitrotoluene

Measured: 2.10

Predicted: 1.72

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2,4-Dinitrotoluene

Measured: 1.98

Predicted: 1.93

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Formaldehyde, (2,4-dinitrophenyl)hydrazone

Measured: 2.33

Predicted: 2.08