

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 202 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.74e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

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2-Methyl-4,6-dinitrophenol

Measured: 257

Predicted: 125

Image not found

3-Trifluoromethyl-4-nitrophenol

Measured: 129

Predicted: 219

Image not found

3,5-Dinitroaniline

Measured: 355

Predicted: 311

Image not found

Safrole

Measured: 676

Predicted: 79.7

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3,5-Dinitrobenzoic acid

Measured: 33.9

Predicted: 70.8