

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
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 11.0

**Global applicability domain:** Inside

**Local applicability domain index:** 4.99e-01

**Confidence level:** 8.15e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

1,2-Dibromoethane

**Measured:** 15.1

**Predicted:** 13.4

[Image not found](#)

Isoprene

**Measured:** 20.0

**Predicted:** 15.6

[Image not found](#)

Bromoform

**Measured:** 13.5

**Predicted:** 14.5

[Image not found](#)

Thiophene, 3-methyl-

**Measured:** 5.25

**Predicted:** 7.49

[Image not found](#)

1,3-Dinitrobenzene

**Measured:** 5.89

**Predicted:** 10.5