

2,4,6-Tricyano-1,3,5-triazine
7615-57-8 | DTXSID00274764

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.76e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.78e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Malonic acid, dihydrazide

Measured: 7.57e-01

Predicted: 5.26e-01

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5-Amino-1,3-dimethyl-6-sulfanylidenedihydropyrimidine-2,4(1H,3H)-dione

Measured: 7.64e-02

Predicted: 7.29e-02

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1,3-Thiazole-2-carbohydrazide

Measured: 2.10e-01

Predicted: 9.13e-02

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N,N'-Dimethyl-N-cyanoacetylurea

Measured: 1.48

Predicted: 9.56e-01