

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 6.88

Global applicability domain: Inside

Local applicability domain index: 9.93e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

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1,5-Dichloronaphthalene

Measured: 6.65

Predicted: 6.90

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1,4-Dichloronaphthalene

Measured: 6.78

Predicted: 6.90

[Image not found](#)

2,7-Dichloronaphthalene

Measured: 6.70

Predicted: 6.90

[Image not found](#)

trans-Stilbene

Measured: 7.48

Predicted: 6.90

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Fluorene

Measured: 6.79

Predicted: 7.07