

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.49e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.48e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

Image not found

Hexachloropropene

Measured: 5.70e-07

Predicted: 3.67e-01

Image not found

2-(Diisopropylamino)ethanol

Measured: 8.49e-05

Predicted: 2.32e-01

Image not found

Dicloran

Measured: 6.44e-06

Predicted: 4.17e-06

Image not found

Benzoyl chloride

Measured: 9.00e-04

Predicted: 3.80e-01

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1-Methyl-2-(propan-2-yl)benzene

Measured: 4.55e-05

Predicted: 1.09