

Triethylenetetramine
112-24-3 | DTXSID9023702

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.435

Global applicability domain: Inside

Local applicability domain index: 4.07e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

Image not found

4,4-Dimethyl-3-thiosemicarbazide

Measured: -0.300

Predicted: -0.357

Image not found

N,N-Diethylhydrazinecarboxamide

Measured: -0.620

Predicted: -0.733

Image not found

N-Nitrosopiperazine

Measured: 0.18

Predicted: -0.0453

Image not found

Dinotefuran

Measured: -0.644

Predicted: -0.450

Image not found

Dinitrosopiperazine

Measured: -0.850

Predicted: -0.682