

Ethanimidic acid, N-hydroxy-, ethyl ester
10576-12-2 | DTXSID2065129

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 3.25 °C

Global applicability domain: Inside

Local applicability domain index: 5.65e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

Image not found

Acetamide, N-acetyl-N-methyl-

Measured: -25.0

Predicted: -28.7

Image not found

Acetoxime

Measured: 61.0

Predicted: 37.2

Image not found

Diethylcarbamoyl chloride

Measured: -32.0

Predicted: -25.5

Image not found

N,N-Dimethylacetamide

Measured: -20.0

Predicted: -31.7