

1,4-Dideoxy-1,4-iminothreitol
90481-32-6 | DTXSID50238179

Model Performance

Model	Data
-------	------

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: 75.4 °C

Global applicability domain: Inside

Local applicability domain index: 4.59e-01

Confidence level: 5.14e-01

Nearest Neighbors from the Training Set

Image not found

2-Amino-2-ethyl-1,3-propanediol

Measured: 37.5

Predicted: 43.0

Image not found

1,3-Propanediol, 2-amino-2-methyl-

Measured: 110

Predicted: 84.6

Image not found

Diethanolamine

Measured: 28.0

Predicted: 32.8

Image not found

Diisopropanolamine

Measured: 44.5

Predicted: 46.5

Image not found

p-Synephrine

Measured: 185

Predicted: 163