

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 6.41

Global applicability domain: Outside

Local applicability domain index: 1.46e-01

Confidence level: 5.62e-01

Nearest Neighbors from the Training Set

Image not found

Salicylic acid

Measured: 7.44

Predicted: 7.60

Image not found

4-Hydroxybenzoic acid

Measured: 8.08

Predicted: 7.78

Image not found

Cyclohexanol

Measured: 5.18

Predicted: 4.72

Image not found

1-Hexanol

Measured: 5.18

Predicted: 4.67

Image not found

Dipropylamine

Measured: 3.59

Predicted: 4.37