

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

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.38 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 6.89e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-(2-Hydroxyethyl)acetamide

Measured: 9.70

Predicted: 9.03

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Diisopropanolamine

Measured: 6.49

Predicted: 7.15

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Noxytiolin [INN:BAN:DCF]

Measured: 8.32e-01

Predicted: N/A

[Image not found](#)

N-Methyldiethanolamine

Measured: 8.39

Predicted: 8.36

[Image not found](#)

Diethanolamine

Measured: 9.51

Predicted: 9.35