

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.10 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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Maleic hydrazide

Measured: 2.82

Predicted: 5.12

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2,2'-Bioxirane

Measured: 2.51

Predicted: 4.97

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Amitrole

Measured: 17.8

Predicted: 10.6

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Diethanolamine

Measured: 3.98

Predicted: 4.00

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1,2-Propylene glycol

Measured: 2.29

Predicted: 4.24