

2,2-Dimethylpropane-1,3-diol
126-30-7 | DTXSID8027036

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: 10.7 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.06e-01

Confidence level: 7.23e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Butanediol

Measured: 11.1

Predicted: 11.3

Image not found

1,2-Butanediol

Measured: 11.1

Predicted: 11.3

Image not found

2,3-Butanediol

Measured: 11.1

Predicted: 9.94

Image not found

1,4-Butanediol

Measured: 11.1

Predicted: 10.2

Image not found

2-Methyl-2,4-pentanediol

Measured: 8.46

Predicted: 3.58