

2-(Hydroxymethyl)-2-methyl-1,3-propanediol
77-85-0 | DTXSID2026444

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: 5.35e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.57e-01

Confidence level: 5.46e-01

Nearest Neighbors from the Training Set

Image not found

Glycerol

Measured: 10.9

Predicted: 6.96

Image not found

Propionic acid, 3,3'-diselenodi-

Measured: 5.39e-03

Predicted: 1.65e-02

Image not found

1,3-Butanediol

Measured: 11.1

Predicted: 11.3