

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.876

Global applicability domain: Inside

Local applicability domain index: 5.65e-01

Confidence level: 5.75e-01

Nearest Neighbors from the Training Set

Image not found

2-Ethyl-2-(hydroxymethyl)-1,3-propanediol

Measured: -1.48

Predicted: -1.17

Image not found

2,3-Butanediol

Measured: -0.920

Predicted: -0.560

Image not found

2-Methylpropane-1,3-diol

Measured: 0.24

Predicted: -0.254

Image not found

Pentaerythritol

Measured: -1.69

Predicted: -1.74