

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 12.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 6.69e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diethanolamine

Measured: 3.98

Predicted: 4.00

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6-Methyl-2-thiouracil

Measured: 138

Predicted: 99.5

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Maleic hydrazide

Measured: 2.82

Predicted: 5.12

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1,2-Diethylhydrazine

Measured: 15.1

Predicted: 14.1

[Image not found](#)

1,4-Dioxane

Measured: 17.0

Predicted: 13.2