

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

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 2.13e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.85e-01

Confidence level: 3.95e-01

Nearest Neighbors from the Training Set

Image not found

Sulfuramid

Measured: 3.36e-03

Predicted: 4.42e-06

Image not found

Heptanedioic acid

Measured: 2.80e-04

Predicted: 1.02e-07

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Triallylamine

Measured: 3.59e-06

Predicted: 2.91

Image not found

Glycerol

Measured: 1.68e-04

Predicted: 1.31e-04

Image not found

Diisobutylamine

Measured: 1.25e-04

Predicted: 11.4