

2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

Model Performance

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

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: 1.29

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 7.20e-01

Nearest Neighbors from the Training Set

Image not found

2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.24

Predicted: 1.29

Image not found

Sobrepin

Measured: 1.81

Predicted: 2.06

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(2,2,6,6-Tetramethyl-4-oxopiperidin-1-yl)oxidanyl

Measured: 0.12

Predicted: 1.95e-01