

3-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-1-ol
6318-30-5 | DTXSID40282782

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: 9.41e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 3.63e-01

Nearest Neighbors from the Training Set

Image not found

Decanal

Measured: 2.19e-02

Predicted: 1.51e-01

Image not found

Tetraethylenepentamine

Measured: 1.18e-03

Predicted: 1.09e-06

Image not found

1-Octanethiol

Measured: 1.26e-01

Predicted: 3.49e-01

Image not found

Quinuclidine

Measured: 107

Predicted: 2.06

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Heptanal

Measured: 2.50e-01

Predicted: 2.33