

2,2-Dimethylpropane-1,3-diol
126-30-7 | DTXSID8027036

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.94e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.25e-01

Confidence level: 6.24e-01

Nearest Neighbors from the Training Set

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2-Butanethiol

Measured: 2.10e-01

Predicted: 67.6

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Hexylamine

Measured: 3.90e-03

Predicted: 16.4

Image not found

2-Methylpentane

Measured: 2.01e-02

Predicted: 127

Image not found

Pentanal

Measured: 1.05e-02

Predicted: 33.1

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6-Aminoquinoline

Measured: 5.01e-02

Predicted: 1.68e-04