

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.44

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

Image not found

2,2-Dimethylpropane-1,3-diol

Measured: 4.68

Predicted: 4.44

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Thiourea

Measured: 2.00

Predicted: 2.11

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Dimethyl sulfoxide

Measured: 3.98

Predicted: 4.07

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1,1'-Oxybis-2-propanol

Measured: 4.57

Predicted: 3.83

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Sulfolane

Measured: 7.08

Predicted: 6.91