

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.12×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.96×10^{-1}

Confidence level: 7.56×10^{-1}

Nearest Neighbors from the Training Set

Image not found

3-Methoxybutan-1-ol

Measured: 2.36×10^{-11}

Predicted: 2.52×10^{-11}

Image not found

Dimethylaminoethanol

Measured: 9.00×10^{-11}

Predicted: 4.44×10^{-11}

Image not found

2-Amino-2-methylpropan-1-ol

Measured: 2.80×10^{-11}

Predicted: 2.88×10^{-11}

Image not found

3-Ethoxy-1-propanol

Measured: 2.20×10^{-11}

Predicted: 2.14×10^{-11}

Image not found

2-Propoxyethanol

Measured: 2.14×10^{-11}

Predicted: 2.14×10^{-11}