

1,3-diphenylpropane-1,2-diol
5381-84-0 | DTXSID50281584

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: 2.84

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

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

Measured: 1.00

Predicted: 1.47

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Oxydisulfoton

Measured: 1.00

Predicted: 1.63

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O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35

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Menthol

Measured: 10.8

Predicted: 23.5

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(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5