

3,4-Dihydroxyacetophenone
1197-09-7 | DTXSID30152546

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: 1.84e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 4.33e-01

Nearest Neighbors from the Training Set

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4-Isopropylphenol

Measured: 1.92e-07

Predicted: 3.08e-02

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1,2-Benzenedicarbonyl
dichloride

Measured: 6.36e-07

Predicted: 2.89e-03

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1,4-Diisopropylbenzene

Measured: 9.20e-06

Predicted: 4.52e-01

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N,N-Dimethylformamide

Measured: 8.20e-05

Predicted: 5.14

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2-Dodecanone

Measured: 6.67e-07

Predicted: 2.01e-02