

(1,1'-Biphenyl)-2,2'-diol
1806-29-7 | DTXSID6051809

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.41e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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1,5-Dihydroxynaphthalene

Measured: 1.03e-03

Predicted: 8.87e-03

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1,3-Naphthalenediol

Measured: 1.12e-02

Predicted: 2.01e-02

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8-Quinazolinol

Measured: 9.20e-03

Predicted: 2.10e-02

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

Measured: 1.45e-01

Predicted: 2.34e-01