

(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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.63e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.51e-01

Confidence level: 3.06e-01

Nearest Neighbors from the Training Set

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Methylcyclopentane

Measured: 9.75e-11

Predicted: 80.1

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2-Propanone, 1,3-diphenyl-

Measured: 7.53e-06

Predicted: 3.07e-04

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Hydroprene

Measured: 3.39e-09

Predicted: 8.80e-04

Image not found

Phenyl glycidyl ether

Measured: 4.36e-04

Predicted: 1.23e-02

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Fenuron

Measured: 1.21e-05

Predicted: 1.82e-05