

2-Hydroxy-3-methylbenzoic acid

83-40-9 | DTXSID9038686

Model Performance

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: 1.30e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.71e-01

Confidence level: 4.66e-01

Nearest Neighbors from the Training Set

Image not found

N,N-Dimethylformamide

Measured: 8.20e-05

Predicted: 5.14

Image not found

4-Isopropylphenol

Measured: 1.92e-07

Predicted: 3.08e-02

Image not found

Chloridazon

Measured: 1.20e-05

Predicted: 1.36e-07

Image not found

1,2-Benzenedicarbonyl
dichloride

Measured: 6.36e-07

Predicted: 2.89e-03

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3-Phenyl-1-propanol

Measured: 2.21e-03

Predicted: 5.06e-02