

Salicylic acid
69-72-7 | DTXSID7026368

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: 2.08e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.74e-01

Confidence level: 4.22e-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

1,2-Benzenedicarbonyl
dichloride

Measured: 6.36e-07

Predicted: 2.89e-03

Image not found

Chloridazon

Measured: 1.20e-05

Predicted: 1.36e-07

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2-Methylbenzothiazole

Measured: 3.66e-03

Predicted: 2.57e-02