

Phenoxyacetic acid
122-59-8 | DTXSID9025873

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: 6.36e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.51e-01

Confidence level: 3.99e-01

Nearest Neighbors from the Training Set

Image not found

2,6-Diethylaniline

Measured: 1.59e-05

Predicted: 2.02e-02

Image not found

4-(2,4-Dinitroanilino)phenol

Measured: 3.43e-02

Predicted: 1.31e-11

Image not found

Butyl phenyl ether

Measured: 1.08e-03

Predicted: 5.92e-01

Image not found

2-Methoxyprop-1-ene

Measured: 8.46e-02

Predicted: 474

Image not found

Isopentyl benzoate

Measured: 5.90e-06

Predicted: 4.01e-02