

1,2-Dichlorobenzene
95-50-1 | DTXSID6020430

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: 1.31 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.65e-01

Confidence level: 8.42e-01

Nearest Neighbors from the Training Set

Image not found

2,4-D 1-butyl ester

Measured: 1.36

Predicted: 3.93e-05

Image not found

o-Cresol

Measured: 3.43

Predicted: 2.70e-01

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2,4-Dichlorotoluene

Measured: 3.15e-01

Predicted: 4.96e-01

Image not found

2,4-Dimethylaniline

Measured: 4.58e-01

Predicted: 1.11e-01

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N-tert-Butyl-2-benzothiazolesulfenamide

Measured: 6.61

Predicted: 2.66e-07