

1-Chloronaphthalene
90-13-1 | DTXSID2024791

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: 1.45e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.75e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

Image not found

1-Methylnaphthalene

Measured: 2.90e-02

Predicted: 2.13e-02

Image not found

2-Methylnaphthalene

Measured: 1.22e-02

Predicted: 2.48e-02

Image not found

1-Methoxy-2-nitrobenzene

Measured: 8.93e-03

Predicted: 6.33e-03

Image not found

Tripropylamine

Measured: 2.46e-03

Predicted: 4.93