

1-Phenylurea
64-10-8 | DTXSID8042507

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: 4.65e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.96e-01

Confidence level: 4.52e-01

Nearest Neighbors from the Training Set

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N-Methylaniline

Measured: 2.60e-02

Predicted: 2.12e-01

[Image not found](#)

Chloroneb

Measured: 5.53e-04

Predicted: 7.69e-03

[Image not found](#)

1-Undecene

Measured: 2.46e-03

Predicted: 3.07e-01

[Image not found](#)

4-Isopropylphenol

Measured: 1.92e-07

Predicted: 3.08e-02

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Sulfallate

Measured: 2.06e-03

Predicted: 1.01e-03