

Urea, (m-fluorophenyl)-
770-19-4 | DTXSID40227815

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: 2.54e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.86e-01

Confidence level: 3.29e-01

Nearest Neighbors from the Training Set

Image not found

4-Isopropylphenol

Measured: 1.92e-07

Predicted: 3.08e-02

Image not found

N,N-Dimethylformamide

Measured: 8.20e-05

Predicted: 5.14

Image not found

N-Methylaniline

Measured: 2.60e-02

Predicted: 2.12e-01

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1,2-Benzenedicarbonyl
dichloride

Measured: 6.36e-07

Predicted: 2.89e-03

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Naphthalene, 1,2,4,7-tetrachloro-

Measured: 3.45e-10

Predicted: 1.23e-05