

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.20e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.61e-01

Confidence level: 5.71e-01

Nearest Neighbors from the Training Set

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2(1H)-Pyrimidinone

Measured: 4.73

Predicted: 2.97

[Image not found](#)

5-ethyl-5-methyl-1,3-oxazolidine-
2,4-dione

Measured: 1.05

Predicted: 6.87e-01

[Image not found](#)

Quinoxalin-5(1H)-one

Measured: 4.50e-02

Predicted: 9.62e-02

[Image not found](#)

4(1H)-Pyrimidinone

Measured: 3.85

Predicted: 2.25

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2-
Cyclohexylidenehydrazinecarboxamide

Measured: 3.87e-02

Predicted: 8.20e-02