

Urea, (3-methylphenyl)-
63-99-0 | DTXSID1075351

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: 1.17e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.50e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

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Quinoxalin-5(1H)-one

Measured: 4.50e-02

Predicted: 9.62e-02

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2-

Cyclohexylidenehydrazinecarboxamide

Measured: 3.87e-02

Predicted: 8.20e-02

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2-Amino-1-ethyl-1,5-dihydro-4H-

imidazol-4-one

Measured: 6.84e-01

Predicted: 5.00e-01

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Tranid

Measured: 8.28e-03

Predicted: 1.40e-02

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4(1H)-Pyrimidinone

Measured: 3.85

Predicted: 2.25