

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.20

Global applicability domain: Inside

Local applicability domain index: 5.77e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

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1-Phenylurea

Measured: 0.83

Predicted: 1.20

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Urea, (3-methylphenyl)-

Measured: 1.29

Predicted: 1.08

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(2-Chlorophenyl)urea

Measured: 1.27

Predicted: 1.76

[Image not found](#)

3-Chlorophenylurea

Measured: 1.82

Predicted: 1.93

[Image not found](#)

Urea, 1-(p-fluorophenyl)-

Measured: 1.04

Predicted: 1.08