

Urea, 1-(p-fluorophenyl)-
659-30-3 | DTXSID20216106

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: 1.08

Global applicability domain: Inside

Local applicability domain index: 6.87e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

Image not found

Urea, 1-(p-fluorophenyl)-

Measured: 1.04

Predicted: 1.08

Image not found

Urea, (m-fluorophenyl)-

Measured: 1.29

Predicted: 1.07

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Urea, (3-methylphenyl)-

Measured: 1.29

Predicted: 1.08

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(2-Fluorophenyl)urea

Measured: 0.88

Predicted: 8.30e-01

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Benzylurea

Measured: 0.73

Predicted: 2.26e-01