

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 49.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.47e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Urea, 1-(p-fluorophenyl)-

Measured: 33.1

Predicted: 49.6

[Image not found](#)

Urea, (m-fluorophenyl)-

Measured: 58.9

Predicted: 59.1

[Image not found](#)

(2-Fluorophenyl)urea

Measured: 20.9

Predicted: 52.8

[Image not found](#)

4-Aminobenzoic acid

Measured: 316

Predicted: 96.6

[Image not found](#)

3-Chlorophenylurea

Measured: 102

Predicted: 57.3