

3-Bromophenylurea
2989-98-2 | DTXSID70184008

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: 1.98

Global applicability domain: Inside

Local applicability domain index: 5.83e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

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3-Bromophenylurea

Measured: 2.08

Predicted: 1.98

[Image not found](#)

(3-Methyl-4-bromophenyl)urea

Measured: 2.49

Predicted: 2.03

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N-(4-Bromophenyl)urea

Measured: 1.98

Predicted: 1.98

[Image not found](#)

3-Chlorophenylurea

Measured: 1.82

Predicted: 1.93

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(2-Chlorophenyl)urea

Measured: 1.27

Predicted: 1.76