

Benzoic acid, 3,6-dichloro-2-hydroxy-
3401-80-7 | DTXSID9041657

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: 4.98e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.74e-01

Confidence level: 5.07e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Acetyl-methionine

Measured: 1.07

Predicted: 5.88e-01

[Image not found](#)

Quinoline-5-carboxylic acid

Measured: 2.10e-03

Predicted: 7.19e-02

[Image not found](#)

Hippuric acid

Measured: 2.09e-02

Predicted: 1.54e-01