

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 274 °C

Global applicability domain: Inside

Local applicability domain index: 2.47e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

Image not found

2-Hydroxyphenylacetic acid

Measured: 240

Predicted: 261

Image not found

2,5-Dichlorobenzoic acid

Measured: 301

Predicted: 288

Image not found

1-Naphthalenecarboxylic acid,
3,4-dihydro-

Measured: 306

Predicted: 300