

Urochloralic acid
97-25-6 | DTXSID30242658

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: 305 °C

Global applicability domain: Outside

Local applicability domain index: 1.36e-01

Confidence level: 5.34e-01

Nearest Neighbors from the Training Set

Image not found

Pyrogallol

Measured: 309

Predicted: 292

Image not found

Erythritol

Measured: 331

Predicted: 327

Image not found

Triisopropanolamine

Measured: 305

Predicted: 302

Image not found

2-Hydroxyphenylacetic acid

Measured: 240

Predicted: 261

Image not found

Triethanolamine

Measured: 335

Predicted: 326