

2,3,6-Trichlorophenylacetic acid sodium salt
2439-00-1 | DTXSID4041319

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 157 °C

Global applicability domain: Inside

Local applicability domain index: 9.07e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

Image not found

Chlorfenac

Measured: 161

Predicted: 157

Image not found

2,3,5-Trichlorobenzoic acid

Measured: 167

Predicted: 157

Image not found

2,4,5-Trichlorobenzoic acid

Measured: 167

Predicted: 158

Image not found

2,3,6-Trichlorobenzoic acid

Measured: 125

Predicted: 151

Image not found

2,4,6-Trichlorobenzoic acid

Measured: 162

Predicted: 157