

Niclosamide
50-65-7 | DTXSID7040362

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: 343 °C

Global applicability domain: Outside

Local applicability domain index: 1.91e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 2-phenylhydrazide

Measured: 314

Predicted: 306

Image not found

3,3'-Dimethoxybenzidine

Measured: 356

Predicted: 361

Image not found

4,4'-Methylenebis(2-chloroaniline)

Measured: 379

Predicted: 361

Image not found

3,3'-Dichlorobenzidine

Measured: 368

Predicted: 361

Image not found

2-Acetylaminofluorene

Measured: 303

Predicted: 340