

Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt
946-30-5 | DTXSID4061339

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: 184 °C

Global applicability domain: Inside

Local applicability domain index: 3.72e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethoxzolamide

Measured: 189

Predicted: 193

[Image not found](#)

4-(4-Methoxybenzoyl)thiophene-
2-sulfonamide

Measured: 174

Predicted: 180

[Image not found](#)

Benazolin

Measured: 193

Predicted: 188