

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.90e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.34e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Benzenesulfonic acid, 3-hydrazino-

Measured: 1.49e-01

Predicted: 5.98e-01

[Image not found](#)

1H-Imidazole-2-sulfonic acid

Measured: 8.44e-01

Predicted: 7.41e-01

[Image not found](#)

1H-Imidazole-5-sulfonic acid

Measured: 1.35

Predicted: 7.40e-01

[Image not found](#)

2-(2,4-Dichlorophenoxy)ethyl hydrogen sulfate

Measured: 8.71e-01

Predicted: 4.28e-01