

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.726

Global applicability domain: Inside

Local applicability domain index: 4.94e-01

Confidence level: 4.57e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Mesylaniline

Measured: -0.120

Predicted: -0.565

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Benzenesulfonic acid, 3-amino-,
monosodium salt

Measured: -3.40

Predicted: -2.10

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4-Aminobenzenesulfonic acid

Measured: -2.16

Predicted: -2.12

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p-(Methylsulphonyl)benzoic acid

Measured: 0.67

Predicted: 5.52e-01