

2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid  
5445-04-5 | DTXSID30396827

### 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
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 6.51

**Global applicability domain:** Inside

**Local applicability domain index:** 2.62e-01

**Confidence level:** 7.28e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Sodium 3-nitrobenzenesulfonate

**Measured:** 5.01

**Predicted:** 5.24

[Image not found](#)

Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

**Measured:** 3.02

**Predicted:** 5.14

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Benzenesulfonic acid, 2,5-dichloro-4-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)-

**Measured:** 32.4

**Predicted:** 9.93

[Image not found](#)

2-Amino-5-methylbenzenesulfonic acid

**Measured:** 3.98

**Predicted:** 6.29

[Image not found](#)

4-Amino-1-naphthalenesulfonic acid sodium salt

**Measured:** 6.03

**Predicted:** 5.38