

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.22e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.46e-01

Confidence level: 2.51e-01

Nearest Neighbors from the Training Set

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Buminafos [ISO]

Measured: 2.30e-11

Predicted: 3.69e-04

Image not found

Sulcotrione

Measured: 1.73e-08

Predicted: 2.68e-08

Image not found

p,p'-DDE

Measured: 4.46e-11

Predicted: 2.89e-06

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Naphthalene, 1,2,4,7-tetrachloro-

Measured: 3.45e-10

Predicted: 1.23e-05