

# PUBCHEM\_54609806

3698-87-1 | DTXSID60715027

## 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:** 6.13e-01

**Global applicability domain:** Inside

**Local applicability domain index:** 2.21e-01

**Confidence level:** 9.24e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

2-Amino-5-methylbenzenesulfonic acid

**Measured:** 0.6

**Predicted:** 7.98e-01

[Image not found](#)

Sodium 3-nitrobenzenesulfonate

**Measured:** 0.7

**Predicted:** 7.21e-01

[Image not found](#)

2-Amino-1-naphthalenesulfonic acid

**Measured:** 0.78

**Predicted:** 8.06e-01

[Image not found](#)

4-Amino-1-naphthalenesulfonic acid sodium salt

**Measured:** 0.78

**Predicted:** 7.49e-01

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Tris(2-hydroxyethyl)isocyanurate

**Measured:** 0.2

**Predicted:** 2.08e-01