

2-Amino-5-methylbenzenesulfonic acid  
88-44-8 | DTXSID7026526

### Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

#### 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:** 1.98e-01 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 3.92e-01

**Confidence level:** 5.53e-01

## Nearest Neighbors from the Training Set

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4-Aminobenzenesulfonic acid

**Measured:** 6.24e-02

**Predicted:** 1.78e-01

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Benzenesulfonic acid, 3-amino-4-methoxy-

**Measured:** 1.26e-01

**Predicted:** 1.74e-01

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Taurocyamine

**Measured:** 2.33e-01

**Predicted:** 3.13e-01

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Benzenesulfonic acid, 3-hydrazino-

**Measured:** 1.49e-01

**Predicted:** 5.98e-01