

Methanesulfonic acid
75-75-2 | DTXSID4026422

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.95 | 0.69 | 0.95 | 0.65 | 0.96 | 0.68 |

Model Results

Predicted value: 4.10

Global applicability domain: Inside

Local applicability domain index: 9.82e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

Image not found

Pyrrrolidine

Measured: 4.07

Predicted: 4.10

Image not found

1-Butanol

Measured: 4.19

Predicted: 4.03

Image not found

Butylamine

Measured: 3.61

Predicted: 4.09

Image not found

2-Chloroethanol

Measured: 4.30

Predicted: 4.07

Image not found

Isopentyl alcohol

Measured: 4.52

Predicted: 4.24