

2-Amino-1-naphthalenesulfonic acid
81-16-3 | DTXSID7020922

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 |

Model Results

Predicted value: 305 °C

Global applicability domain: Outside

Local applicability domain index: 1.70e-01

Confidence level: 5.01e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Trimellitic anhydride

Measured: 390

Predicted: 366

[Image not found](#)

Chloramben

Measured: 312

Predicted: 301

[Image not found](#)

Diphenylurea

Measured: 262

Predicted: 269

[Image not found](#)

Benzoic acid, 2-benzoyl-

Measured: 261

Predicted: 309