

1H-Imidazole-2-sulfonic acid
53744-47-1 | DTXSID40601515

Model Performance

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

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: 2.95e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.49e-01

Confidence level: 3.56e-01

Nearest Neighbors from the Training Set

Image not found

Chlorthion

Measured: 2.00e-08

Predicted: 6.17e-06

Image not found

beta-Ionone

Measured: 9.80e-08

Predicted: 5.46e-02

Image not found

Furalaxyl

Measured: 1.13e-06

Predicted: 3.22e-07

Image not found

Propane, 1-ethoxy-

Measured: 7.49e-07

Predicted: 138