

1H-Imidazole-5-sulfonic acid
60634-74-4 | DTXSID80524673

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: 225 °C

Global applicability domain: Inside

Local applicability domain index: 3.56e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

[Image not found](#)

I-Taurine

Measured: 328

Predicted: 295

[Image not found](#)

5-Carboxy-2-thiouracil

Measured: 252

Predicted: 236

[Image not found](#)

Fluridamid

Measured: 176

Predicted: 183

[Image not found](#)

4-Imidazolidinone, 2-thioxo-

Measured: 230

Predicted: 220

[Image not found](#)

Primocarcin

Measured: 131

Predicted: 143