

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 225 °C

Global applicability domain: Inside

Local applicability domain index: 3.54e-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