

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

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.588

Global applicability domain: Inside

Local applicability domain index: 4.42e-01

Confidence level: 5.71e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Pyrimidine-2-carbothioamide

Measured: -0.340

Predicted: 9.67e-02

[Image not found](#)

Pyrimidine-2-thiol

Measured: -1.11

Predicted: -0.822