

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

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.40e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.68e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found

Taurocyamine

Measured: 2.33e-01

Predicted: 3.13e-01

Image not found

I-Taurine

Measured: 6.45e-01

Predicted: 8.59e-01

Image not found

1H-Imidazole-2-sulfonic acid

Measured: 8.44e-01

Predicted: 7.41e-01

Image not found

1H-Imidazole-5-sulfonic acid

Measured: 1.35

Predicted: 7.40e-01

Image not found

5-Methyl-1H-imidazole-4-sulfonic acid

Measured: 1.54

Predicted: 7.96e-01