

6-Mercaptopurine
50-44-2 | DTXSID0020810

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.51

Global applicability domain: Inside

Local applicability domain index: 4.45e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

Image not found

Amitrole

Measured: 3.09

Predicted: 3.40

Image not found

Ethylene thiourea

Measured: 1.82

Predicted: 1.85

Image not found

N,N-Dimethylformamide

Measured: 7.94e-01

Predicted: 1.12

Image not found

Morpholine

Measured: 2.82

Predicted: 1.87

Image not found

1,4-Dioxane

Measured: 5.01e-01

Predicted: 1.06