

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.46e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.04e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

Image not found

2,4-Dinitrotoluene

Measured: 2.21e-08

Predicted: 2.66e-04

Image not found

Chlorothalonil

Measured: 2.89e-07

Predicted: 1.44e-06

Image not found

Methidathion

Measured: 9.98e-07

Predicted: 3.29e-06

Image not found

cis-Nonachlordane

Measured: 1.20e-09

Predicted: 2.30e-06

Image not found

Terbacil

Measured: 1.12e-06

Predicted: 9.25e-07