

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
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 343 °C

**Global applicability domain:** Outside

**Local applicability domain index:** 2.16e-01

**Confidence level:** 5.77e-01

## Nearest Neighbors from the Training Set

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**Measured:** 345

**Predicted:** 341

Image not found

3-Methyl-1-phenyl-1H-pyrazol-5-amine

**Measured:** 333

**Predicted:** 334

Image not found

1,2,3-Benzotriazole

**Measured:** 350

**Predicted:** 294

Image not found

Ametryn

**Measured:** 345

**Predicted:** 341

Image not found

1,2,4-Triaminobenzene

**Measured:** 340

**Predicted:** 315