

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
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 31.3 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 4.61e-01

**Confidence level:** 6.53e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

6-Methyl-2-thiouracil

**Measured:** 138

**Predicted:** 99.5

[Image not found](#)

6-Chloro-2-picolinic acid

**Measured:** 23.4

**Predicted:** 53.1

[Image not found](#)

Maleic hydrazide

**Measured:** 2.82

**Predicted:** 5.12

[Image not found](#)

Phthalic anhydride

**Measured:** 36.3

**Predicted:** 38.0