

Nitrofurantoin
67-20-9 | DTXSID7020972

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: 6.89e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.88e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Metharbital

Measured: 9.99e-03

Predicted: 1.04e-02

[Image not found](#)

Nitrofurantoin

Measured: 3.34e-04

Predicted: 6.89e-03

[Image not found](#)

1-Methylcarbamoyl-5-fluorouracil

Measured: 3.31e-03

Predicted: 6.11e-03