

Hexamethylphosphoramide
680-31-9 | DTXSID6020694

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: 3.41 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 6.22e-01

Nearest Neighbors from the Training Set

Image not found

Hexamethylphosphoramide

Measured: 5.58

Predicted: 3.41

Image not found

Dimefox

Measured: 6.49

Predicted: 4.15

Image not found

Cyclophosphamide

Measured: 1.53e-01

Predicted: 8.08e-02

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Mipafox

Measured: 4.39e-01

Predicted: 4.12e-01