

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: 4.15 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.46e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Dimefox

Measured: 6.49

Predicted: 4.15

[Image not found](#)

Mipafox

Measured: 4.39e-01

Predicted: 4.12e-01

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Hexamethylphosphoramide

Measured: 5.58

Predicted: 3.41

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Ethyl dimethyl phosphate

Measured: 3.24

Predicted: 3.42