

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: 2.47 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.86e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Monocrotophos

Measured: 4.48

Predicted: 2.47

[Image not found](#)

Dicrotophos

Measured: 4.22

Predicted: 2.95

[Image not found](#)

cis-Mevinphos

Measured: 4.46

Predicted: 3.48