

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: 1120 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.98e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

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Disulfoton

Measured: 1660

Predicted: 1120

[Image not found](#)

Phorate

Measured: 501

Predicted: 588

[Image not found](#)

Terbufos

Measured: 661

Predicted: 623

[Image not found](#)

Terbufos sulfoxide

Measured: 151

Predicted: 239

[Image not found](#)

Fonofos

Measured: 871

Predicted: 759