

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.25

Global applicability domain: Inside

Local applicability domain index: 4.15e-01

Confidence level: 4.47e-01

Nearest Neighbors from the Training Set

Image not found

Malathion

Measured: 2.36

Predicted: 2.29

Image not found

Tris(2-chloroethyl) phosphate

Measured: 1.44

Predicted: 1.58

Image not found

Heptenophos

Measured: 2.32

Predicted: 2.25

Image not found

Dichlorvos

Measured: 1.43

Predicted: 1.25

Image not found

Propetamphos

Measured: 3.82

Predicted: 3.21