

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 330 °C

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Dieldrin

Measured: 330

Predicted: 330

[Image not found](#)

(+/-)-Oxychlordane

Measured: 353

Predicted: 346

[Image not found](#)

Heptachlor

Measured: 310

Predicted: 319