

Model Performance

Model	Data
-------	------

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: 313 °C

Global applicability domain: Outside

Local applicability domain index: 2.96e-01

Confidence level: 5.58e-01

Nearest Neighbors from the Training Set

Image not found

Tris(2-chloroethyl) phosphate

Measured: 330

Predicted: 316

Image not found

Heptachlor

Measured: 310

Predicted: 319

Image not found

(+/-)-Oxychlorane

Measured: 353

Predicted: 346

Image not found

Phenyl phosphorodichloridate

Measured: 242

Predicted: 255

Image not found

Dieldrin

Measured: 330

Predicted: 330