

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: 156 °C

Global applicability domain: Inside

Local applicability domain index: 5.67e-01

Confidence level: 6.16e-01

Nearest Neighbors from the Training Set

Image not found

Sarin

Measured: 147

Predicted: 156

Image not found

Trimethyl phosphate

Measured: 197

Predicted: 185

Image not found

Dimethyl methylphosphonate

Measured: 181

Predicted: 173

Image not found

Trimethyl phosphite

Measured: 112

Predicted: 131

Image not found

Diethyl methanephosphonate

Measured: 194

Predicted: 193