

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.65 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.51e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

Image not found

Sarin

Measured: 7.14

Predicted: 1.65

Image not found

Cyclosarin

Measured: 2.05e-02

Predicted: 5.91e-02

Image not found

Pinacolyl

methylphosphonofluoridate

Measured: 1.15e-01

Predicted: 1.33e-01

Image not found

Diisopropyl fluorophosphate

Measured: 8.36e-02

Predicted: 8.23e-02

Image not found

Ethyl 4,4,4-trifluoroacetoacetate

Measured: 4.35e-02

Predicted: 7.99e-02