

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: 3.86e-01

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 5.56e-01

Nearest Neighbors from the Training Set

Image not found

Sarin

Measured: 0.3

Predicted: 3.86e-01

Image not found

Diethyl ethylphosphonate

Measured: 0.66

Predicted: 6.30e-01

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Phosphonic acid, bis(1-methylethyl) ester

Measured: 0.45

Predicted: 5.25e-01

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Diisopropyl methylphosphonate

Measured: 1.03

Predicted: 1.40

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Propane, 1,1'-sulfonylbis-

Measured: 0.39

Predicted: 5.67e-01