

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.13e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.29e-01

Confidence level: 4.38e-01

Nearest Neighbors from the Training Set

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p,p'-DDE

Measured: 4.46e-11

Predicted: 2.89e-06

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2,4-Dinitrotoluene

Measured: 2.21e-08

Predicted: 2.66e-04

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Pirimiphos-ethyl

Measured: 2.00e-06

Predicted: 2.79e-05

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Chlorothalonil

Measured: 2.89e-07

Predicted: 1.44e-06

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Limonene

Measured: 1.31e-07

Predicted: 1.32

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D-Limonene

Measured: 1.31e-07

Predicted: 1.32

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(S)-Limonene

Measured: 1.31e-07

Predicted: 1.32

