

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: 1.61e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.98e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

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Isoprocarb

Measured: 7.88e-04

Predicted: 8.64e-05

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Fenthion

Measured: 1.05e-05

Predicted: 3.98e-05

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Etridiazole

Measured: 2.60e-06

Predicted: 6.47e-04

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Phorate

Measured: 7.50e-05

Predicted: 2.45e-04

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Phenmedipham

Measured: 1.58e-05

Predicted: 2.47e-10