

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: 7.15e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

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2,4,5-Trichlorophenoxyacetic acid

Measured: 1.50e-05

Predicted: 4.08e-06

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Fluazuron

Measured: 7.57e-05

Predicted: 1.00e-09

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Methyl benzoate

Measured: 6.16e-05

Predicted: 3.32e-01

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Diphenylurea

Measured: 1.50e-04

Predicted: 1.72e-06

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Acetylugenol

Measured: 2.32e-04

Predicted: 6.51e-04