

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: 1.70e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.55e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

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1-Methyl phenanthrene

Measured: 2.74e-06

Predicted: 1.84e-05

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Cycloundecanone

Measured: 1.69e-06

Predicted: 2.62e-02

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Methidathion

Measured: 9.98e-07

Predicted: 3.29e-06

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Phenol, 4-chloro-5-methyl-2-nitro-

Measured: 1.24e-06

Predicted: 3.85e-03

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Acetophenone, 3-ethyl-

Measured: 1.40e-06

Predicted: 3.43e-01