

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: 1.54e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 4.53e-01

Nearest Neighbors from the Training Set

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Benzoic acid, 3,5-dimethoxy-

Measured: 2.00e-03

Predicted: 1.18e-05

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Benzene, octyl-

Measured: 5.60e-03

Predicted: 1.26e-02

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Pentachloropyridine

Measured: 1.50e-04

Predicted: 9.68e-04

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2,4-D, Dimethylamine salt

Measured: 1.30e-02

Predicted: 7.12e-07

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Secbumeton

Measured: 3.68e-05

Predicted: 3.61e-06