

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: 4.72e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.72e-01

Confidence level: 3.64e-01

Nearest Neighbors from the Training Set

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Diphacinone

Measured: 5.00e-05

Predicted: 2.11e-10

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Hexachloropropene

Measured: 5.70e-07

Predicted: 3.67e-01

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9,10-Anthracenedione, 1-amino-4-hydroxy-

Measured: 1.80e-03

Predicted: 3.75e-09

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Diethyl phthalate

Measured: 1.80e-05

Predicted: 3.30e-07