

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: 4.06e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.71e-01

Confidence level: 4.99e-01

Nearest Neighbors from the Training Set

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Dimethoate

Measured: 4.20e-06

Predicted: 1.70e-05

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Thiophene, 2-bromo-

Measured: 1.95e-05

Predicted: 11.9

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Propanedinitrile, dimethyl-

Measured: 2.00e-07

Predicted: 1.16e-01

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Cyclodecane

Measured: 2.92e-06

Predicted: 4.64e-01

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Chlordane

Measured: 2.05e-05

Predicted: 2.03e-05

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cis-Chlordane

Measured: 2.05e-05

Predicted: 2.03e-05

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trans-Chlordane

Measured: 2.05e-05

Predicted: 2.03e-05

[Image not found](#)

Chlordane

Measured: 2.05e-05

Predicted: 2.03e-05

