

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: 7.03 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.38e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

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Ethylenediamine

Measured: 26.1

Predicted: 6.61

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2-Methylpent-1-ene

Measured: 3.55

Predicted: 61.0

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Barbituric acid

Measured: 6.70

Predicted: 4.85e-08

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1-Propanol

Measured: 2.20

Predicted: 21.3

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1,2-Dichloroethane

Measured: 7.18

Predicted: 99.3