

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: 7.05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 7.34e-01

Nearest Neighbors from the Training Set

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Pentyl mercaptan

Measured: 10.1

Predicted: 17.5

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Tetradecylbenzene

Measured: 1.70

Predicted: 1.52e-05

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Pirimicarb

Measured: 1.30

Predicted: 5.21e-06

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2-Butenoic acid

Measured: 12.5

Predicted: 2.74e-01

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2-Amino-3-chloro-1,4-naphthoquinone

Measured: 3.12

Predicted: 3.50e-07