

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: 268 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.53e-01

Confidence level: 8.55e-01

Nearest Neighbors from the Training Set

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Dodecylbenzene

Measured: 317

Predicted: 7.09e-05

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Arecoline

Measured: 232

Predicted: 1.33e-01

[Image not found](#)

Paraldehyde

Measured: 111

Predicted: 7.30

[Image not found](#)

Acetonitrile

Measured: 902

Predicted: 61.0

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2-Methyl-1-propanol

Measured: 173

Predicted: 10.5