

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:** 1.59e-01 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 8.45e-01

**Confidence level:** 8.75e-01

## Nearest Neighbors from the Training Set

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Triethylenetetramine

**Measured:** 1.35e-01

**Predicted:** 2.46e-04

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Decanoic acid

**Measured:** 2.08e-01

**Predicted:** 9.27e-04

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Bis-(2-chloroethyl)sulfide

**Measured:** 2.08e-01

**Predicted:** 6.99e-01

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1-Methyl-2-propylbenzene

**Measured:** 4.12e-01

**Predicted:** 1.10

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Octane, 1-iodo-

**Measured:** 5.58e-02

**Predicted:** 1.82e-01