

Model Performance

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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:** 1.49e-01 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.00e-01

**Confidence level:** 5.06e-01

## Nearest Neighbors from the Training Set

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Cyclobutane, octafluoro-

**Measured:** 1.10e-01

**Predicted:** 3340

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1-Propene, 3,3,3-trifluoro-

**Measured:** 4.60e-02

**Predicted:** 3540

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2-Pentene, 3-methyl-

**Measured:** 4.69e-02

**Predicted:** 156

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N-Nitrosodiethylamine

**Measured:** 8.60e-01

**Predicted:** 1.48

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2,3-Dimethylbutan-2-ol

**Measured:** 12.0

**Predicted:** 5.17