

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:** 5360 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 8.37e-01

**Confidence level:** 6.74e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Octadecane

**Measured:** 2850

**Predicted:** 1.51e-04

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Phosgene

**Measured:** 7250

**Predicted:** 1080

[Image not found](#)

1,1-Difluoroethane

**Measured:** 30000

**Predicted:** 3310

[Image not found](#)

2-Piperidone

**Measured:** 4390

**Predicted:** 1.80e-02

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Acetyl chloride

**Measured:** 4550

**Predicted:** 95.8