

Model Performance

Model	Data
-------	------

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:** 1.96e-02 mmHg

**Global applicability domain:** Outside

**Local applicability domain index:** 3.17e-01

**Confidence level:** 2.52e-01

## Nearest Neighbors from the Training Set

Image not found

Bensulide

**Measured:** 2.48e-01

**Predicted:** 1.34e-06

Image not found

Benazolin

**Measured:** 4.28e-07

**Predicted:** 8.30e-09

Image not found

2-Butene, 1,1,1,2,3,4,4,4-octafluoro-

**Measured:** 1.33e-01

**Predicted:** 2800

Image not found

1-Propene, 3-propoxy-

**Measured:** 0.1

**Predicted:** 64.5

Image not found

Silane, chlorodimethylphenyl-

**Measured:** 2.91

**Predicted:** 1.01