

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: 2.67e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.70e-01

Confidence level: 2.14e-01

Nearest Neighbors from the Training Set

Image not found

2,3-Benzofluorene

Measured: 1.35e-04

Predicted: 2.22e-07

Image not found

Triphenylene

Measured: 2.08e-05

Predicted: 1.87e-08

Image not found

Fluorene

Measured: 7.50e-07

Predicted: 9.71e-04

Image not found

Dimefox

Measured: 3.98e-07

Predicted: 1.49e-01