

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: 1.45e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.06e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

Image not found

Fenchol

Measured: 9.80e-06

Predicted: 6.35e-02

Image not found

(1R)-endo-(+)-Fenchyl alcohol

Measured: 9.80e-06

Predicted: 6.35e-02

Image not found

N,N-Dimethylaniline

Measured: 3.38e-06

Predicted: 4.54e-01

Image not found

Flubenzimine

Measured: 8.00e-05

Predicted: 2.90e-06

Image not found

Chloroacetaldehyde

Measured: 2.60e-04

Predicted: 81.8