

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: 2.84e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.77e-01

Confidence level: 7.88e-01

Nearest Neighbors from the Training Set

Image not found

Triacotane

Measured: 2.40e-06

Predicted: 8.27e-11

Image not found

Daminozide

Measured: 2.90e-06

Predicted: 2.23e-05

Image not found

Iprobenfos

Measured: 7.30e-06

Predicted: 1.52e-05

Image not found

2,4-Dichlorobiphenyl

Measured: 2.00e-06

Predicted: 1.51e-03

Image not found

1,1'-Biphenyl, 4,4'-dinitro-

Measured: 2.30e-06

Predicted: 8.64e-08