

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: 8.52e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 4.17e-01

Nearest Neighbors from the Training Set

Image not found

Acetone

Measured: 8.76e-10

Predicted: 262

Image not found

2-Methoxy-3,4-dihydro-2H-pyran

Measured: 1.00e-11

Predicted: 4.87

Image not found

Oct-2-yne

Measured: 5.00e-11

Predicted: 10.3

Image not found

Acetic acid, 2,2-dichloro-, methyl ester

Measured: 3.00e-09

Predicted: 11.5