

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: 9.19e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.21e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

Image not found

1-Naphthol

Measured: 2.56e-04

Predicted: 2.28e-04

Image not found

beta-Pinene

Measured: 4.18e-03

Predicted: 2.53

Image not found

Ethylenediaminetetraacetic acid

Measured: 1.40e-06

Predicted: 2.81e-12

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Benzene, 1,1'-ethenylidenebis-

Measured: 4.91e-04

Predicted: 1.69e-02

Image not found

Methyl salicylate

Measured: 5.27e-06

Predicted: 4.27e-03