

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.77

Global applicability domain: Inside

Local applicability domain index: 4.13e-01

Confidence level: 4.67e-01

Nearest Neighbors from the Training Set

[Image not found](#)

5,6-Dihydrocyclopenta[c]
[1,2]dithiole-3(4H)-thione

Measured: 2.53

Predicted: 2.55

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Benzodithiolone

Measured: 2.73

Predicted: 2.04

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2,4,6-Tribromoresorcinol

Measured: 4.37

Predicted: 2.57