

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.05 days

Global applicability domain: Inside

Local applicability domain index: 5.15e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

Image not found

5-Methylindan

Measured: 4.93

Predicted: 2.25

Image not found

9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A

Image not found

4-Methylindan

Measured: 4.93

Predicted: 2.31

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1H-Indene, 2-methyl-

Measured: 12.5

Predicted: 2.48

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3-Methylindene

Measured: 12.5

Predicted: 2.76