

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: 3.55 days

Global applicability domain: Outside

Local applicability domain index: 3.43e-01

Confidence level: 9.35e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17

Image not found

Propylbenzene

Measured: 24.3

Predicted: 4.02

Image not found

3-Ethyltoluene

Measured: 12.5

Predicted: 3.26

Image not found

4-Ethyltoluene

Measured: 24.3

Predicted: 3.95

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1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89