

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: 3.73 days

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 9.13e-01

Nearest Neighbors from the Training Set

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1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89

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1,2-Dimethyl-4-ethylbenzene

Measured: 40.7

Predicted: 4.08

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4-Ethyltoluene

Measured: 24.3

Predicted: 3.95

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3-Ethyltoluene

Measured: 12.5

Predicted: 3.26

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2-Ethyl-p-xylene

Measured: 12.5

Predicted: 3.70