

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:** 12.4 days

**Global applicability domain:** Outside

**Local applicability domain index:** 3.61e-01

**Confidence level:** 7.71e-01

## Nearest Neighbors from the Training Set

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Cumene

**Measured:** 511

**Predicted:** 11.8

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Hexane, 2,2,5-trimethyl-

**Measured:** 777

**Predicted:** 17.4

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Isobutylbenzene

**Measured:** 201

**Predicted:** 6.97

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1,2-Dimethylcyclohexane

**Measured:** 777

**Predicted:** 10.2