

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
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 28.0

**Global applicability domain:** Inside

**Local applicability domain index:** 3.64e-01

**Confidence level:** 6.01e-01

## Nearest Neighbors from the Training Set

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1,2-Difluoro-1,1,2,2-tetrachloroethane

**Measured:** 58.9

**Predicted:** 37.2

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1,1-Dichloroethylene

**Measured:** 12.9

**Predicted:** 9.95

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1-Chloro-4-nitrobenzene

**Measured:** 20.0

**Predicted:** 12.2

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1-Chloro-2-nitrobenzene

**Measured:** 14.8

**Predicted:** 22.1

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1-Chloro-3-nitrobenzene

**Measured:** 77.6

**Predicted:** 15.9