

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:** 4.19

**Global applicability domain:** Inside

**Local applicability domain index:** 5.31e-01

**Confidence level:** 6.65e-01

## Nearest Neighbors from the Training Set

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Diethyl ether

**Measured:** 5.37

**Predicted:** 4.72

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tert-Butyl alcohol

**Measured:** 5.01

**Predicted:** 4.48

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2-Nitropropane

**Measured:** 8.32

**Predicted:** 7.41

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1,4-Dioxane

**Measured:** 5.01e-01

**Predicted:** 1.06

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4-Methylimidazolidine-2-thione

**Measured:** 10.0

**Predicted:** 4.59