

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:** 4.36

**Global applicability domain:** Inside

**Local applicability domain index:** 2.47e-01

**Confidence level:** 7.00e-01

## Nearest Neighbors from the Training Set

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Benzoic acid, 4-(methylamino)-

**Measured:** 2.40

**Predicted:** 4.00

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Benzilic acid

**Measured:** 1.82

**Predicted:** 3.42

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2,2-Dimethylpropanoic acid

**Measured:** 2.29

**Predicted:** 2.74

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Benzenesulfonic acid, 2,5-dichloro-4-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)-

**Measured:** 32.4

**Predicted:** 9.93

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Phenylphosphinic acid

**Measured:** 6.03

**Predicted:** 4.42