

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:** 2.92

**Global applicability domain:** Inside

**Local applicability domain index:** 4.08e-01

**Confidence level:** 8.43e-01

## Nearest Neighbors from the Training Set

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Benzenesulfonamide

**Measured:** 4.79

**Predicted:** 2.10

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o-Toluenesulfonamide

**Measured:** 2.57

**Predicted:** 2.00

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Sulfolane

**Measured:** 7.08

**Predicted:** 6.91

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Triethyl phosphate

**Measured:** 1.29

**Predicted:** 1.38

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Trimethyl phosphate

**Measured:** 1.41

**Predicted:** 1.50