

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:** 53.0

**Global applicability domain:** Outside

**Local applicability domain index:** 2.34e-01

**Confidence level:** 6.50e-01

## Nearest Neighbors from the Training Set

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Benzotrifluoride

**Measured:** 44.7

**Predicted:** 13.7

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2,4-Dichlorobenzotrifluoride

**Measured:** 2340

**Predicted:** 108

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3-Chlorobenzotrifluoride

**Measured:** 224

**Predicted:** 317

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1,1,1,3,3,3-Hexafluoro-2-propanol

**Measured:** 2.51

**Predicted:** 2.40

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Dichlorodifluoromethane

**Measured:** 6.17

**Predicted:** 9.03