

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
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 4.23

**Global applicability domain:** Inside

**Local applicability domain index:** 3.61e-01

**Confidence level:** 3.84e-01

## Nearest Neighbors from the Training Set

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Perflenapent

**Measured:** 4.40

**Predicted:** 4.23

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3,3,4,4,5,5,6,6,7,7,8,8,8-  
Tridecafluorooctan-1-ol

**Measured:** 4.54

**Predicted:** 4.45

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1-Hexanol, 3,3,4,4,5,5,6,6,6-  
nonafluoro-

**Measured:** 3.30

**Predicted:** 3.01

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1,1,2,2-Tetrahydroperfluoro-1-  
decanol

**Measured:** 5.58

**Predicted:** 5.05

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2,4-Dimethyl-1-octylpyridin-1-ium  
iodide

**Measured:** -0.570

**Predicted:** 3.81