

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:** -0.646

**Global applicability domain:** Inside

**Local applicability domain index:** 5.64e-01

**Confidence level:** 6.06e-01

## Nearest Neighbors from the Training Set

Image not found

Morpholine

**Measured:** -0.860

**Predicted:** -0.646

Image not found

Ethanamine, N-methyl-

**Measured:** 0.15

**Predicted:** 1.26e-01

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1,4-Dioxane

**Measured:** -0.270

**Predicted:** -0.157

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Piperazine

**Measured:** -1.50

**Predicted:** -1.20

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N-Methyl-N-propylamine

**Measured:** 0.84

**Predicted:** 7.94e-01