

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: 10.1

Global applicability domain: Inside

Local applicability domain index: 4.45e-01

Confidence level: 5.33e-01

## Nearest Neighbors from the Training Set

Image not found

Molinate

**Measured:** 25.7

**Predicted:** 14.8

Image not found

Phenacetin

**Measured:** 30.2

**Predicted:** 3.76

Image not found

Menthol

**Measured:** 10.8

**Predicted:** 23.5

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(1R,2S,5R)-(-)-Menthol

**Measured:** 10.8

**Predicted:** 23.5

Image not found

4-Isobutylmorpholine

**Measured:** 1.78

**Predicted:** 2.69