

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:** 7.48

**Global applicability domain:** Outside

**Local applicability domain index:** 1.25e-01

**Confidence level:** 7.16e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

2,5-Pyridinedicarboxylic acid

**Measured:** 5.75

**Predicted:** 4.09

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Benzenesulfonic acid, 2,5-dichloro-4-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)-

**Measured:** 32.4

**Predicted:** 9.93

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Docosate sodium

**Measured:** 9.33

**Predicted:** 8.95