

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
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 4.61e-05 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 4.49e-01

**Confidence level:** 4.18e-01

## Nearest Neighbors from the Training Set

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Captafol

**Measured:** 4.01e-06

**Predicted:** 1.43e-05

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Thioperoxydiphosphoric acid  
([(HO)2P(S)]2S2), tetramethyl  
ester

**Measured:** 4.00e-05

**Predicted:** 7.24e-05

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Captan

**Measured:** 1.70e-05

**Predicted:** 4.23e-05

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Benquinox

**Measured:** 2.07e-05

**Predicted:** 3.02e-02

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1-Benzoylazepan-2-one

**Measured:** 6.81e-03

**Predicted:** 1.14e-01