

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:** 2.59e-01

**Global applicability domain:** Inside

**Local applicability domain index:** 4.02e-01

**Confidence level:** 5.93e-01

## Nearest Neighbors from the Training Set

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MLS003389292

**Measured:** 0.02

**Predicted:** 2.24e-01

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N,N,N',N'-Tetramethyl-P-pyrrolidin-1-ylphosphonic diamide

**Measured:** 0.82

**Predicted:** 7.91e-01

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Uracil, 5-(dimethylamino)-1,3,6-trimethyl-

**Measured:** 0.99

**Predicted:** 8.30e-01

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Tri(aziridin-1-yl)phosphine oxide

**Measured:** -0.620

**Predicted:** -0.469