

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
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 419 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.61e-01

**Confidence level:** 7.47e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Cycloate

**Measured:** 347

**Predicted:** 419

[Image not found](#)

Diallate

**Measured:** 1910

**Predicted:** 1430

[Image not found](#)

Butylate

**Measured:** 129

**Predicted:** 358

[Image not found](#)

Pebulate

**Measured:** 631

**Predicted:** 430

[Image not found](#)

Vernolate

**Measured:** 214

**Predicted:** 379