

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: 204 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.75e-01

Confidence level: 7.36e-01

Nearest Neighbors from the Training Set

Image not found

EPTC

Measured: 240

Predicted: 204

Image not found

Vernolate

Measured: 214

Predicted: 379

Image not found

Molinate

Measured: 83.2

Predicted: 219

Image not found

Butylate

Measured: 129

Predicted: 358

Image not found

Pebulate

Measured: 631

Predicted: 430