

### 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	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 4.50e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 3.88e-01

**Confidence level:** 7.42e-01

## Nearest Neighbors from the Training Set

Image not found

Cycloate

**Measured:** 3.54e-11

**Predicted:** 2.98e-11

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EPTC

**Measured:** 3.18e-11

**Predicted:** 2.83e-11

Image not found

Triethyl phosphate

**Measured:** 5.53e-11

**Predicted:** 4.26e-11

Image not found

2-(2-Butoxyethoxy)ethanol

**Measured:** 7.44e-11

**Predicted:** 5.15e-11