

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:**  $7.02 \times 10^{-13}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $2.85 \times 10^{-1}$

**Confidence level:**  $8.63 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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2,2',3,5',6-Pentachlorobiphenyl

**Measured:**  $4.00 \times 10^{-13}$

**Predicted:**  $1.72 \times 10^{-11}$

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2,3,3',4',6-Pentachlorobiphenyl

**Measured:**  $6.00 \times 10^{-13}$

**Predicted:**  $1.72 \times 10^{-11}$

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2,2',3,5'-tetrachlorobiphenyl

**Measured:**  $8.00 \times 10^{-13}$

**Predicted:**  $3.33 \times 10^{-11}$

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2,2',4,4'-Tetrachlorobiphenyl

**Measured:**  $1.00 \times 10^{-12}$

**Predicted:**  $3.31 \times 10^{-11}$