

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:** 2.75e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 2.76e-01

**Confidence level:** 7.10e-01

## Nearest Neighbors from the Training Set

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1,4-Benzoquinone

**Measured:** 4.60e-12

**Predicted:** 5.97e-12

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2-Methyl-p-benzoquinone

**Measured:** 2.35e-11

**Predicted:** 2.15e-11

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1,3,5-Cycloheptatriene

**Measured:** 9.69e-11

**Predicted:** 1.00e-10

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(2E)-3-Phenylprop-2-enal

**Measured:** 4.80e-11

**Predicted:** 5.31e-11