

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: 2.83e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

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EPTC

Measured: 3.18e-11

Predicted: 2.83e-11

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Cycloate

Measured: 3.54e-11

Predicted: 2.98e-11

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Simazine

Measured: 1.10e-11

Predicted: 1.22e-11

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Triethyl phosphate

Measured: 5.53e-11

Predicted: 4.26e-11

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p-Nitroanisole

Measured: 2.46e-12

Predicted: 1.65e-11