

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: 1.12e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.12e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Naphthoquinone

Measured: 3.10e-12

Predicted: 3.16e-11

Image not found

2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11

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2,5-Furandione

Measured: 1.45e-12

Predicted: 2.17e-12