

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: 3.64e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 7.02e-01

Nearest Neighbors from the Training Set

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Dimefox

Measured: 6.40e-11

Predicted: 3.64e-11

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O,S,S-Trimethyl
phosphorodithioate

Measured: 9.59e-12

Predicted: 1.50e-11

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N-Methylcarbamic acid, ethyl
ester

Measured: 8.30e-12

Predicted: 1.01e-11

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Carbamic acid, ethyl-, methyl
ester

Measured: 1.05e-11

Predicted: 1.06e-11

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Phosphoramidic acid, dimethyl-,
dimethyl ester

Measured: 3.19e-11

Predicted: 2.75e-11