

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: 2.10e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

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Dimefox

Measured: 6.40e-11

Predicted: 3.64e-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

[Image not found](#)

Ethyl ethylcarbamate

Measured: 1.44e-11

Predicted: 1.58e-11

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Triethyl phosphate

Measured: 5.53e-11

Predicted: 4.26e-11