

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: 2.32e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.74e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

Image not found

2-Ethoxyethanol

Measured: 1.54e-11

Predicted: 1.51e-11

Image not found

Diethoxymethane

Measured: 1.68e-11

Predicted: 1.95e-11

Image not found

Ethylene glycol diethyl ether

Measured: 5.79e-11

Predicted: 3.42e-11

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1-Methoxy-2-propanol

Measured: 1.86e-11

Predicted: 1.93e-11