

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: 3.61×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.47×10^{-1}

Confidence level: 8.04×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Furfural

Measured: 3.51×10^{-11}

Predicted: 5.73×10^{-11}

Image not found

2-Furancarboxaldehyde, 5-methyl-

Measured: 5.10×10^{-11}

Predicted: 4.23×10^{-11}

Image not found

3-Furaldehyde

Measured: 4.85×10^{-11}

Predicted: 5.07×10^{-11}

Image not found

n-Butoxyacetaldehyde

Measured: 2.06×10^{-11}

Predicted: 2.17×10^{-11}