

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: 2.08e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.73e-01

Confidence level: 9.51e-01

Nearest Neighbors from the Training Set

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Propanal

Measured: 1.96e-11

Predicted: 2.08e-11

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2-Methylpropanal

Measured: 2.63e-11

Predicted: 2.53e-11

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Butyraldehyde

Measured: 2.35e-11

Predicted: 2.45e-11

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Acetaldehyde

Measured: 1.58e-11

Predicted: 1.52e-11

Image not found

Pentanal

Measured: 2.85e-11

Predicted: 2.79e-11