

Acetaldehyde
75-07-0 | DTXSID5039224

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: 1.52×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.13×10^{-1}

Confidence level: 8.16×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Acetaldehyde

Measured: 1.58×10^{-11}

Predicted: 1.52×10^{-11}

Image not found

Propanal

Measured: 1.96×10^{-11}

Predicted: 2.08×10^{-11}

Image not found

Chloroacetaldehyde

Measured: 3.10×10^{-12}

Predicted: 4.01×10^{-12}

Image not found

2-Methylpropanal

Measured: 2.63×10^{-11}

Predicted: 2.53×10^{-11}

Image not found

Butyraldehyde

Measured: 2.35×10^{-11}

Predicted: 2.45×10^{-11}