

Hydrogen cyanide
74-90-8 | DTXSID9024148

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: 3.80×10^{-14} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 1.77×10^{-1}

Confidence level: 4.59×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Hydrogen cyanide

Measured: 3.00×10^{-14}

Predicted: 3.80×10^{-14}

Image not found

Formaldehyde

Measured: 9.37×10^{-12}

Predicted: 5.67×10^{-12}

Image not found

Formyl chloride

Measured: 3.20×10^{-13}

Predicted: 2.22×10^{-13}

Image not found

Dibromomethane

Measured: 1.13×10^{-13}

Predicted: 7.92×10^{-14}

Image not found

Chloromethane

Measured: 4.36×10^{-14}

Predicted: 4.65×10^{-14}