

Formaldehyde

50-00-0 | DTXSID7020637

Model Performance

Model

Data

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: -11.2 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.32e-01

Confidence level: 4.50e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Formaldehyde

Measured: -11.0

Predicted: -11.2

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Hydrogen cyanide

Measured: -13.5

Predicted: -13.4

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Formyl chloride

Measured: -12.5

Predicted: -12.7

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HFC-41

Measured: -13.8

Predicted: -13.4

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Dibromomethane

Measured: -12.9

Predicted: -13.1