

Cyclopropane--water (1/1)
26163-08-6 | DTXSID10737557

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: -24.5 °C

Global applicability domain: Inside

Local applicability domain index: 7.05e-01

Confidence level: 6.84e-01

Nearest Neighbors from the Training Set

Image not found

Cyclopropane

Measured: -32.8

Predicted: -24.5

Image not found

Vinyl chloride

Measured: -13.3

Predicted: -15.4

Image not found

1-Propene

Measured: -48.0

Predicted: -35.4

Image not found

Ethylene oxide

Measured: 10.6

Predicted: 11.9

Image not found

Ethyl methyl ether

Measured: 7.40

Predicted: 14.4