

Methyl acetate
79-20-9 | DTXSID4021767

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -89.6 °C

Global applicability domain: Inside

Local applicability domain index: 7.74e-01

Confidence level: 8.47e-01

Nearest Neighbors from the Training Set

Image not found

Methyl acetate

Measured: -98.0

Predicted: -89.6

Image not found

Ethyl formate

Measured: -79.6

Predicted: -87.5

Image not found

Methyl propanoate

Measured: -87.5

Predicted: -86.1

Image not found

Ethyl acetate

Measured: -83.6

Predicted: -86.0

Image not found

Formic acid, propyl ester

Measured: -92.9

Predicted: -87.2