

Propanoic acid, 2-(1-oxopropoxy)-, methyl ester
61402-72-0 | DTXSID30485366

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: -23.1 °C

Global applicability domain: Inside

Local applicability domain index: 8.72e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl propanedioate

Measured: -50.0

Predicted: -34.4

Image not found

Dimethyl glutarate

Measured: -42.5

Predicted: -25.9

Image not found

Dimethyl adipate

Measured: 10.3

Predicted: -9.04

Image not found

Diethyl butanedioate

Measured: -21.0

Predicted: -13.4