

Ethyl lactate
97-64-3 | DTXSID6029127

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: -16.9 °C

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 3.02e-01

Nearest Neighbors from the Training Set

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Methyl 2-hydroxypropanoate

Measured: -66.0

Predicted: -52.7

Image not found

Butyl lactate

Measured: -28.0

Predicted: -17.5

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Acetoin

Measured: 15.0

Predicted: -4.20

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1-Methoxy-2-propanol

Measured: -95.0

Predicted: -55.4

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3-Ethoxy-1-propanol

Measured: 161

Predicted: 42.9