

Ethyl lactate
97-64-3 | DTXSID6029127

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.16

Global applicability domain: Inside

Local applicability domain index: 9.51e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

Image not found

1-Pentanol

Measured: 4.69

Predicted: 4.17

Image not found

Piperidine

Measured: 4.04

Predicted: 4.32

Image not found

Isopentyl alcohol

Measured: 4.52

Predicted: 4.24

Image not found

Dipropylamine

Measured: 3.59

Predicted: 4.37

Image not found

Butylamine

Measured: 3.61

Predicted: 4.09