

Ethyl 4-ethoxybutyrate

26448-91-9 | DTXSID10403149

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.31

Global applicability domain: Inside

Local applicability domain index: 9.59e-01

Confidence level: 7.59e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dichlorobenzene

Measured: 4.46

Predicted: 4.45

Image not found

Hexachloroethane

Measured: 4.47

Predicted: 4.45

Image not found

1,3-Dichlorobenzene

Measured: 4.12

Predicted: 4.44

Image not found

1,2-Dichlorobenzene

Measured: 4.36

Predicted: 4.46

Image not found

Propylbenzene

Measured: 4.09

Predicted: 4.53