

4-Butoxybutanoic acid
55724-73-7 | DTXSID90204272

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.51e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found

(Cyclopentyloxy)acetic acid

Measured: 1.42e-01

Predicted: 1.96e-01

Image not found

Propionic acid, 2-(cyclohexyloxy)-2-methyl-

Measured: 8.32e-02

Predicted: 6.22e-02

Image not found

6-Aminocaproic acid

Measured: 3.85

Predicted: 4.69