

2-METHYLHEXANEDIOIC ACID
33659-32-4 | DTXSID20334839

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 323 °C

Global applicability domain: Outside

Local applicability domain index: 6.68e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

Image not found

Heptanedioic acid

Measured: 342

Predicted: 332

Image not found

Hexanedioic acid

Measured: 338

Predicted: 330

Image not found

3-Ethyl-3-methylglutaric acid

Measured: 261

Predicted: 286

Image not found

Octanedioic acid

Measured: 346

Predicted: 332

Image not found

Pentanedioic acid

Measured: 303

Predicted: 310