

2-hydroxy-2,4,4-trimethylpentanoic acid
5438-26-6 | DTXSID90280379

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 239 °C

Global applicability domain: Inside

Local applicability domain index: 2.77e-01

Confidence level: 3.39e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Hydroxyisobutyric acid

Measured: 212

Predicted: 214

[Image not found](#)

2-Hydroxyphenylacetic acid

Measured: 240

Predicted: 261

[Image not found](#)

Chloral hydrate

Measured: 98.0

Predicted: 123

[Image not found](#)

1-Methylcyclohexanecarboxylic acid

Measured: 234

Predicted: 239