

2-(1-Hydroxy-1-methylethyl-2-methyl-1,3-dioxane
39239-96-8 | DTXSID80192497

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: 214 °C

Global applicability domain: Inside

Local applicability domain index: 6.25e-01

Confidence level: 9.25e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isopentyl lactate

Measured: 202

Predicted: 205

[Image not found](#)

dl-Borneol

Measured: 210

Predicted: 213

[Image not found](#)

alpha-Terpineol

Measured: 219

Predicted: 216

[Image not found](#)

alpha-Terpineol

Measured: 219

Predicted: 216

[Image not found](#)

alpha-Terpineol

Measured: 219

Predicted: 216

[Image not found](#)

Diethylene glycol monoisobutyl ether

Measured: 217

Predicted: 219