

1-Butanol, 3-methoxy-3-methyl-, acetate
103429-90-9 | DTXSID30145852

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: 181 °C

Global applicability domain: Inside

Local applicability domain index: 7.37e-01

Confidence level: 7.41e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate

Measured: 192

Predicted: 191

Image not found

Ethane, 1,1,1-triethoxy-

Measured: 145

Predicted: 162

Image not found

Isobutyric anhydride

Measured: 183

Predicted: 185

Image not found

Formic acid, octyl ester

Measured: 199

Predicted: 192

Image not found

Diethylene glycol diethyl ether

Measured: 188

Predicted: 183