

1-methoxypropan-2-yl 2-methylpropanoate
5436-79-3 | DTXSID40281472

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: 179 °C

Global applicability domain: Inside

Local applicability domain index: 7.38e-01

Confidence level: 7.44e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate

Measured: 192

Predicted: 191

Image not found

Isobutyric anhydride

Measured: 183

Predicted: 185

Image not found

Ethane, 1,1,1-triethoxy-

Measured: 145

Predicted: 162

Image not found

Formic acid, octyl ester

Measured: 199

Predicted: 192

Image not found

Formic acid, heptyl ester

Measured: 178

Predicted: 171