

Pentyl acetate
628-63-7 | DTXSID1027263

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: 147 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 9.41e-01

Nearest Neighbors from the Training Set

Image not found

Butanoic acid, propyl ester

Measured: 143

Predicted: 147

Image not found

Ethyl valerate

Measured: 146

Predicted: 147

Image not found

Butyl propionate

Measured: 147

Predicted: 147

Image not found

Pentyl acetate

Measured: 149

Predicted: 147

Image not found

Methyl hexanoate

Measured: 150

Predicted: 147