

Methyl pivalate
598-98-1 | DTXSID4027234

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: 109 °C

Global applicability domain: Inside

Local applicability domain index: 8.88e-01

Confidence level: 8.94e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methyl pivalate

Measured: 101

Predicted: 109

[Image not found](#)

Ethyl isobutyrate

Measured: 110

Predicted: 113

[Image not found](#)

Isobutyl acetate

Measured: 117

Predicted: 113

[Image not found](#)

Butanoic acid, 3-methyl-, methyl ester

Measured: 117

Predicted: 113

[Image not found](#)

Butan-2-yl acetate

Measured: 112

Predicted: 113