



Fluka: 66130
Supelco: R41-2420

>>Derivative: Me ester

CAS Registry Number: 53955-81-0
Molecular Formula: C₆H₁₂O₂
Molecular Weight: 116.16
Accurate Mass: 116.08373
Percentage Composition: C 62.04%; H 10.41%; O 27.55%
Boiling Point: Bp 115°
Density: d 0.88
Refractive Index: n_D²⁰ 1.3930

>>Derivative: Et ester

Synonym(s): Ethyl 2-methylbutyrate. FEMA 2443

CAS Registry Number: 7452-79-1

Molecular Formula: C₇H₁₄O₂
Molecular Weight: 130.186
Accurate Mass: 130.09938
Percentage Composition: C 64.58%; H 10.84%; O 24.58%
Biological Source: Found in fruits
Use/Importance: Flavouring agent. Used in fruit flavouring
Physical Description: Liq. with apple-like odour
Boiling Point: Bp 133.5°
Density: d₄²⁰ 0.87
Refractive Index: n_D²⁰ 1.3964
Aldrich: 30688-6
Fluka: 66135

>>Derivative: Chloride

CAS Registry Number: 57526-28-0
Extra CAS Registry Numbers(s): 5856-79-1
Molecular Formula: C₅H₉ClO
Molecular Weight: 120.578
Accurate Mass: 120.034192
Percentage Composition: C 49.81%; H 7.52%; Cl 29.40%; O 13.27%
Boiling Point: Bp 115-116°

>>Derivative: Amide

CAS Registry Number: 1113-57-1
Molecular Formula: C₅H₁₁NO
Molecular Weight: 101.148
Accurate Mass: 101.084064
Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%
Physical Description: Cryst. (Et₂O)
Melting Point: Mp 112°

>>Derivative: Nitrile

CAS Registry Number: 18936-17-9
Molecular Formula: C₅H₉N
Molecular Weight: 83.133
Percentage Composition: C 72.24%; H 10.91%; N 16.85%
Boiling Point: Bp 125°

>>Derivative: Anhydride

Molecular Formula: C₁₀H₁₈O₃
Molecular Weight: 186.25
Percentage Composition: C 64.49%; H 9.74%; O 25.77%
Boiling Point: Bp₁₇ 103-104°