



Molecular Weight: 172.267
Accurate Mass: 172.14633
Percentage Composition: C 69.72%; H 11.70%; O 18.58%
Boiling Point: Bp₁₈ 77-79°

>>Derivative: 3-Methylbutyl ester

Synonym(s): 3-Methylbutyl hexanoate. Isopentyl caproate. FEMA 2075

CAS Registry Number: 2198-61-0

Molecular Formula: C₁₁H₂₂O₂

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Use/Importance: Used in fruit flavours and in fragrance. Present in fruits and alcoholic beverages

Boiling Point: Bp 222°

Density: d 0.86

>>Derivative: Hexyl ester

Synonym(s): Hexyl hexanoate. Capryl caproate. Hexyl caproate. FEMA 2568

CAS Registry Number: 6378-65-0

Molecular Formula: C₁₂H₂₄O₂

Molecular Weight: 200.32

Accurate Mass: 200.17763

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

Biological Source: Volatile component from fruit ripening

Use/Importance: Used in fruit flavouring

Physical Description: Liq.

Boiling Point: Bp 245° (208°). Bp₁₃ 116-120°

Density: d₂₀²⁰ 0.86

Refractive Index: n_D²⁰ 1.4249

>>Derivative: (E)-2-Hexenyl ester

Synonym(s): 2-Hexenyl hexanoate. 2-Hexenyl caproate

CAS Registry Number: 53398-86-0

Molecular Formula: C₁₂H₂₂O₂

Molecular Weight: 198.305

Accurate Mass: 198.16198

Percentage Composition: C 72.68%; H 11.18%; O 16.14%

Biological Source: Alarm pheromone of *Riptortus clavatus*

Boiling Point: Bp₃ 79°

>>Derivative: Chloride

CAS Registry Number: 142-61-0

Molecular Formula: C₆H₁₁ClO

Molecular Weight: 134.605

Accurate Mass: 134.049842

Percentage Composition: C 53.54%; H 8.24%; Cl 26.34%; O 11.89%

Boiling Point: Bp 151-153°

Aldrich: 29465-9

Fluka: 21590

Sigma: C1899

>>Derivative: Bromide

CAS Registry Number: 51499-41-3

Molecular Formula: C₆H₁₁BrO

Molecular Weight: 179.056

Accurate Mass: 178.019326

Percentage Composition: C 40.25%; H 6.19%; Br 44.63%; O 8.94%

Boiling Point: Bp 175-176°