



Molecular Weight: 115.175
Accurate Mass: 115.099714
Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%
Melting Point: Mp 100°
Solubility: Mod. sol. hot H₂O

Aldrich: 29339-3

>>**Derivative:** Dimethylamide
Synonym(s): *N,N*-Dimethylhexanamide

CAS Registry Number: 5830-30-8
Molecular Formula: C₈H₁₇NO
Molecular Weight: 143.228
Accurate Mass: 143.131014
Percentage Composition: C 67.09%; H 11.96%; N 9.78%; O 11.17%
Use/Importance: Insect repellent

>>**Derivative:** Anilide

CAS Registry Number: 621-15-8
Molecular Formula: C₁₂H₁₇NO
Molecular Weight: 191.272
Accurate Mass: 191.131014
Percentage Composition: C 75.35%; H 8.96%; N 7.32%; O 8.36%
Physical Description: Prisms (EtOH)
Melting Point: Mp 96°

>>**Derivative:** Nitrile
Synonym(s): Hexanenitrile, 9Cl. Capronitrile. 1-Cyanopentane

CAS Registry Number: 628-73-9
Molecular Formula: C₆H₁₁N
Molecular Weight: 97.16
Accurate Mass: 97.089149
Percentage Composition: C 74.17%; H 11.41%; N 14.42%
Boiling Point: Bp 163.6°. Bp₂₅ 75°
Hazard & Toxicity: LD₅₀ (mus, orl) 463 mg/kg

Aldrich: 16665-0

>>**Derivative:** Anhydride

CAS Registry Number: 2051-49-2
Molecular Formula: C₁₂H₂₂O₃
Molecular Weight: 214.304
Accurate Mass: 214.156895
Percentage Composition: C 67.26%; H 10.35%; O 22.40%
Boiling Point: Bp 254-257°. Bp_{14.5} 143°
Other Data: Stable to aq. carbonates
Aldrich: 19453-0
Fluka: 21580
Sigma: C9009

>>**Derivative:** 2-Methylpropyl ester
Synonym(s): 2-Methylpropyl hexanoate. Isobutyl Caproate. FEMA 2202

CAS Registry Number: 105-79-3

Molecular Formula: C₁₀H₂₀O₂
Molecular Weight: 172.267
Accurate Mass: 172.14633
Percentage Composition: C 69.72%; H 11.70%; O 18.58%
Use/Importance: Flavouring ingredient
Physical Description: Liq