



Refractive Index: n_D^{20} 1.4073

Aldrich: W24391-4

Fluka: 21550

Sigma: C9884

>>**Derivative:** Propyl ester

Synonym(s): Propyl hexanoate. Propyl caproate

CAS Registry Number: 626-77-7

Molecular Formula: $C_9H_{18}O_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Boiling Point: Bp 187° (185.5°)

Density: d_4^{15} 0.86

Refractive Index: n_D^{25} 1.4109

>>**Derivative:** Isopropyl ester

Synonym(s): Isopropyl hexanoate. Isopropyl caproate. FEMA 2950

CAS Registry Number: 2311-46-8

Molecular Formula: $C_9H_{18}O_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Use/Importance: Flavouring ingredient

Boiling Point: Bp 161°. Bp₂ 34°. Bp₁₀₀ 109°

Density: d_4^{26} 0.86

>>**Derivative:** 2-Propenyl ester

Synonym(s): 2-Propenyl hexanoate. Allyl caproate. FEMA 2032

CAS Registry Number: 123-68-2

Molecular Formula: $C_9H_{16}O_2$

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Source/Synthesis: Found in fruits

Use/Importance: Used in artificial pineapple flavourings

Physical Description: Liq. with pineapple odour

Boiling Point: Bp₁₅ 75-76°

Density: d_4^{26} 0.89

Refractive Index: n_D^{20} 1.4243

Aldrich: W20321-1

>>**Derivative:** Butyl ester

Synonym(s): Butyl hexanoate. Butyl caproate

CAS Registry Number: 626-82-4

Molecular Formula: $C_{10}H_{20}O_2$

Molecular Weight: 172.267

Accurate Mass: 172.14633

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Source/Synthesis: Present in fruits and berries

Use/Importance: Used in fruit flavourings

Physical Description: Liq. with powerful fruity odour

Boiling Point: Bp 208°

Refractive Index: n_D^{15} 1.4160

Aldrich: W22010-8