



Supelco: S48-2449

>> **Derivative:** Propyl ester

Synonym(s): Propyl octanoate. Propyl caprylate

CAS Registry Number: 624-13-5

Molecular Formula: C₁₁H₂₂O₂

Molecular Weight: 186.294

Accurate Mass: 186.16198

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

Melting Point: Mp -45°

Boiling Point: Bp 226°

Density: d₄²⁵ 0.86

>> **Derivative:** Isopropyl ester

Synonym(s): Isopropyl octanoate. Isopropyl caprylate

CAS Registry Number: 5458-59-3

Molecular Formula: C₁₁H₂₂O₂

Molecular Weight: 186.294

Accurate Mass: 186.16198

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

Biological Source: Sex pheromone of *Megalophanes viciella*

Physical Description: Oil

Boiling Point: Bp_{0.8} 48-50°

>> **Derivative:** Butyl ester

Synonym(s): Butyl octanoate. Butyl caprylate

CAS Registry Number: 589-75-3

Molecular Formula: C₁₂H₂₄O₂

Molecular Weight: 200.32

Accurate Mass: 200.17763

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

Melting Point: Mp -43°

Boiling Point: Bp 245°

Density: d₂₀²⁰ 0.86

Refractive Index: n_D¹⁵ 1.4232

>> **Derivative:** Pentyl ester

Synonym(s): Pentyl octanoate. Amyl caprylate. FEMA 2079

CAS Registry Number: 638-25-5

Molecular Formula: C₁₃H₂₆O₂

Molecular Weight: 214.347

Accurate Mass: 214.19328

Percentage Composition: C 72.85%; H 12.23%; O 14.93%

Use/Importance: Flavouring agent

Physical Description: Liq

Melting Point: Mp -34--35°

Boiling Point: Bp 260°

Density: d₂₅²⁵ 0.86

Refractive Index: n_D²⁵ 1.4262

>> **Derivative:** Hexyl ester

Synonym(s): Hexyl octanoate. Caproyl caprylate. FEMA 2575

CAS Registry Number: 1117-55-1