



Molecular Formula: C₁₂H₂₂O₂
Molecular Weight: 198.305
Accurate Mass: 198.16198
Percentage Composition: C 72.68%; H 11.18%; O 16.14%
Physical Description: Liq. with a characteristic fruity aroma (cognac, pineapple)
Boiling Point: Bp 230°
Density: d₄³⁶ 0.87
Refractive Index: n_D³⁰ 1.4302
Aldrich: W20360-2

>>Derivative: 4-Bromophenacyl ester

CAS Registry Number: 35300-70-0
Molecular Formula: C₁₇H₂₃BrO₃
Molecular Weight: 355.271
Percentage Composition: C 57.47%; H 6.53%; Br 22.49%; O 13.51%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 68.5°

>>Derivative: Chloride

CAS Registry Number: 764-85-2
Molecular Formula: C₉H₁₇ClO
Molecular Weight: 176.685
Accurate Mass: 176.096792
Percentage Composition: C 61.18%; H 9.70%; Cl 20.07%; O 9.06%
Physical Description: Liq.
Melting Point: Fp -60.5°
Boiling Point: Bp 215°. Bp₁₅ 98°
Aldrich: 15683-3
Fluka: 76360
Sigma: N2629

>>Derivative: Amide
Synonym(s): Nonanamide, 9Cl

CAS Registry Number: 1120-07-6
Molecular Formula: C₉H₁₉NO
Molecular Weight: 157.255
Accurate Mass: 157.146664
Percentage Composition: C 68.74%; H 12.18%; N 8.91%; O 10.17%
Physical Description: Cryst.
Melting Point: Mp 92-93° (98.9°)
Solubility: Insol. cold H₂O
Rare Chemicals Library: S59526-8

>>Derivative: Nitrile
Synonym(s): Nonanenitrile, 9Cl. 1-Cyanooctane. Pelargononitrile. Octyl cyanide

CAS Registry Number: 2243-27-8
Molecular Formula: C₉H₁₇N
Molecular Weight: 139.24
Accurate Mass: 139.136099
Percentage Composition: C 77.64%; H 12.31%; N 10.06%
Physical Description: Liq.
Melting Point: Fp -34.2°
Boiling Point: Bp 224°. Bp₁₅ 102-105°
Refractive Index: n_D²⁰ 1.4260
Hazard & Toxicity: LD₅₀ (mus, orl) 2059 mg/kg

Aldrich: 13126-1
Fluka: 76380

>>Derivative: Anhydride