



Accurate Mass: 196.14633
Percentage Composition: C 73.43%; H 10.27%; O 16.30%
Use/Importance: Used in perfumery. Pineapple flavourant
Physical Description: Liq. with pineapple-like odour
Boiling Point: Bp₁ 91°
Density: d₂₅²⁵ 0.95
Refractive Index: n_D²⁰ 1.4600
Hazard & Toxicity: LD₅₀ (mus, orl) 970-1083 mg/kg

Aldrich: 41165-5

>>Derivative: Ph ester

Molecular Formula: C₁₅H₂₀O₂
Molecular Weight: 232.322
Accurate Mass: 232.14633
Percentage Composition: C 77.55%; H 8.68%; O 13.77%
Boiling Point: Bp₃₁ 195°
Refractive Index: n_D¹⁴ 1.5030

>>Derivative: Chloride

CAS Registry Number: 39098-75-4
Molecular Formula: C₉H₁₅ClO
Molecular Weight: 174.67
Accurate Mass: 174.081142
Percentage Composition: C 61.89%; H 8.66%; Cl 20.30%; O 9.16%
Boiling Point: Bp₃₅ 124-126°. Bp₁₇ 108°

>>Derivative: Amide

CAS Registry Number: 4361-29-9
Molecular Formula: C₉H₁₇NO
Molecular Weight: 155.239
Accurate Mass: 155.131014
Percentage Composition: C 69.63%; H 11.04%; N 9.02%; O 10.31%
Physical Description: Needles (MeOH)
Melting Point: Mp 120°

>>Derivative: Hydrazide

Molecular Formula: C₉H₁₈N₂O
Molecular Weight: 170.254
Accurate Mass: 170.141913
Percentage Composition: C 63.49%; H 10.66%; N 16.45%; O 9.40%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 92°

>>Derivative: Phenylhydrazide

Molecular Formula: C₁₅H₂₂N₂O
Molecular Weight: 246.352
Accurate Mass: 246.173213
Percentage Composition: C 73.13%; H 9.00%; N 11.37%; O 6.49%
Melting Point: Mp 155-156°

References: