



CAS Registry Number: 101-94-0

Molecular Formula: C₁₅H₁₄O₂

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Use/Importance: Used in perfumery

Physical Description: Cryst. with floral odour and sweet honey-like taste

Melting Point: Mp 76° (EtOH)

Boiling Point: Bp 310°

Aldrich: W30771-8

Rare Chemicals Library: S35613-1

>>**Derivative:** 2-Phenylethyl ester

Synonym(s): Phenethyl phenylacetate. 2-Phenylethyl benzeneacetate. FEMA 2866

CAS Registry Number: 102-20-5

Molecular Formula: C₁₆H₁₆O₂

Molecular Weight: 240.301

Accurate Mass: 240.11503

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Use/Importance: Used in perfumery and in imitation fruit flavours

Physical Description: Needles (MeOH) with hyacinth-like odour

Melting Point: Mp 28°

Boiling Point: Bp 325°. Bp₂₈ 210°

>>**Derivative:** Fluoride

Synonym(s): Benzeneacetyl fluoride, 9Cl. Phenacetyl fluoride

CAS Registry Number: 370-84-3

Molecular Formula: C₈H₇FO

Molecular Weight: 138.141

Accurate Mass: 138.048093

Percentage Composition: C 69.56%; H 5.11%; F 13.75%; O 11.58%

Physical Description: Oil

Boiling Point: Bp₁₇ 88-89°

>>**Derivative:** Chloride

Synonym(s): Benzeneacetyl chloride, 9Cl. Phenacetyl chloride

CAS Registry Number: 103-80-0

Molecular Formula: C₈H₇ClO

Molecular Weight: 154.595

Accurate Mass: 154.018542

Percentage Composition: C 62.15%; H 4.56%; Cl 22.93%; O 10.35%

Physical Description: Oil

Boiling Point: Bp₂₅₀ 170°. Bp₁₂ 100°

Density: d₄²⁰ 1.168

Hazard & Toxicity: Irritant. Lachrymator

Aldrich: P1675-3

Fluka: 77830

>>**Derivative:** Bromide

Synonym(s): Benzeneacetyl bromide, 9Cl. Phenacetyl bromide

CAS Registry Number: 22535-03-1

Molecular Formula: C₈H₇BrO

Molecular Weight: 199.047

Accurate Mass: 197.988026

Percentage Composition: C 48.27%; H 3.54%; Br 40.14%; O 8.04%

Physical Description: Oil

Boiling Point: Bp₅₀ 150-155°