



Melting Point: Mp 116° (110-112°)

Aldrich: P1665-6

>>**Derivative:** Nitrile

Synonym(s): Benzeneacetonitrile, 9CI. Benzyl cyanide. Phenylacetonitrile. Benzyl nitrile. Cyanophenylmethane. (Cyanomethyl)benzene

CAS Registry Number: 140-29-4

Molecular Formula: C₈H₇N

Molecular Weight: 117.15

Accurate Mass: 117.057849

Percentage Composition: C 82.02%; H 6.02%; N 11.96%

Biological Source: Isol. from thick-tailed galago *Galago crassicaudatus*, oil of *Lepidium sativum* and other plant oils

Use/Importance: Used in the detection of nitro compds.

Physical Description: Liq.

Boiling Point: Bp 234°. Bp₁₂ 107°

Density: d₁₅¹⁵ 1.021

Refractive Index: n_D²⁵ 1.5211

Hazard & Toxicity: Explosive reaction with NaOCl + H⁽⁺⁾. Skin irritant. LD₅₀ (rat, orl) 270 mg/kg. LD₅₀ (rbt, skn) 270 mg/kg

Aldrich: B1940-1

Fluka: 13300

Sigma: B2890

>>**Derivative:** Anhydride

CAS Registry Number: 1555-80-2

Molecular Formula: C₁₆H₁₄O₃

Molecular Weight: 254.285

Accurate Mass: 254.094295

Percentage Composition: C 75.58%; H 5.55%; O 18.88%

Physical Description: Needles

Melting Point: Mp 72°

>>**Derivative:** Octyl ester

Synonym(s): Octyl phenylacetate. FEMA 2812

CAS Registry Number: 122-45-2

Molecular Formula: C₁₆H₂₄O₂

Molecular Weight: 248.364

Accurate Mass: 248.17763

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Physical Description: Viscous liq.

Boiling Point: Bp 315°

Density: d_{15.5}^{15.5} 0.983

>>**Derivative:** Hexyl ester

Synonym(s): Hexyl phenylacetate

CAS Registry Number: 5421-17-0

Molecular Formula: C₁₄H₂₀O₂

Molecular Weight: 220.311

Accurate Mass: 220.14633

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Use/Importance: Flavouring ingredient

References: