

Phenylacetone

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CambridgeSoft

Monograph Number: 7353

Title: Phenylacetone

CAS Registry Number: 103-79-7

CAS Name: 1-Phenyl-2-propanone

Additional Names: benzyl methyl ketone

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.17.

Percent Composition: C 80.57%, H 7.51%, O 11.92%

Line Formula: C₆H₅CH₂COCH₃

Literature References: Prepn from phenylacetic and acetic acids: R. H. Pickard, J. Kenyon, *J. Chem. Soc.*

105, 1124 (1914); R. M. Herbst, R. H. Manske, *Org. Syn. coll. vol. II*, 389 (1943); from α-

phenylacetoacetonitrile: P. L. Julian, J. J. Oliver, *ibid.* 391; from α-methyl-α-phenylethylene oxide: S. Danilow,

E. Venus-Danilowa, *Ber.* **60**, 1050 (1927); from diethyl malonate: H. G. Walker, C. R. Hauser, *J. Am. Chem.*

Soc. **68**, 1386 (1946). Conformational calculations: M. Hirota *et al.*, *Tetrahedron* **39**, 3091 (1983). Use as

prochiral ketone in enantioselective hydrosilylation: H. Brenner *et al.*, *Ber.* **117**, 1330 (1984).

Properties: Oil, mp -16 to -15°. bp₇₆₀ 214°; bp₁₄ 100-101°. d₄²⁰ 1.0157. n_D 1.5174. uv max (ethanol): 258, 283 nm (ε 255, 150).

Melting point: mp -16 to -15°

Boiling point: bp₇₆₀ 214°; bp₁₄ 100-101°

Index of refraction: n_D 1.5174

Absorption maximum: uv max (ethanol): 258, 283 nm (ε 255, 150)

Density: d₄²⁰ 1.0157

NOTE: This is a controlled substance: **21 CFR**, 1308.12.

Use: In organic synthesis; production of benzyl radicals by photolysis.