



>>Entry Name: 3-Benzoylbenzoic acid, 9CI

Synonym(s): Benzophenone-3-carboxylic acid. Diphenylmethanone-3-carboxylic acid

CAS Registry Number: 579-18-0

Molecular Formula: C₁₄H₁₀O₃

Molecular Weight: 226.231

Accurate Mass: 226.062995

Percentage Composition: C 74.33%; H 4.46%; O 21.22%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 161-162°

Solubility: Spar. sol. H₂O

Other Data: Sublimes

Aldrich: 26179-3

>>Derivative: Me ester

CAS Registry Number: 21204-86-4

Molecular Formula: C₁₅H₁₂O₃

Molecular Weight: 240.258

Accurate Mass: 240.078645

Percentage Composition: C 74.99%; H 5.03%; O 19.98%

Melting Point: Mp 62°

>>Derivative: Chloride

CAS Registry Number: 77301-47-4

Molecular Formula: C₁₄H₉ClO₂

Molecular Weight: 244.677

Accurate Mass: 244.029107

Percentage Composition: C 68.73%; H 3.71%; Cl 14.49%; O 13.08%

Physical Description: Cryst. (hexane)

Melting Point: Mp 49-51°

>>Derivative: Oxime

Molecular Formula: C₁₄H₁₁NO₃

Molecular Weight: 241.246

Accurate Mass: 241.073894

Percentage Composition: C 69.70%; H 4.60%; N 5.81%; O 19.90%

Melting Point: Mp 202.5-203.5°

>>Derivative: Amide, oxime

Molecular Formula: C₁₄H₁₂N₂O₂

Molecular Weight: 240.261

Accurate Mass: 240.089878

Percentage Composition: C 69.99%; H 5.03%; N 11.66%; O 13.32%

Physical Description: Pale yellow cryst.

Melting Point: Mp 194-195°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1166A, (*nmr*)

Smith, M.E., *J.A.C.S.*, 1921, **43**, 1920, (*synth*)

Exner, O. *et al.*, *Coll. Czech. Chem. Comm.*, 1971, **36**, 534, (*ir*)

Ito, Y. *et al.*, *J.O.C.*, 1985, **50**, 2893, (*synth, ir, pmr*)

Maurin, J.K. *et al.*, *Acta Cryst. C*, 1992, **48**, 1821; 2165, (*cryst struct, oximes*)