



>>Entry Name: 4-Benzoylbenzoic acid, 9CI

Synonym(s): Benzophenone-4-carboxylic acid. Diphenylmethanone-4-carboxylic acid

CAS Registry Number: 611-95-0

Molecular Formula: C₁₄H₁₀O₃

Molecular Weight: 226.231

Accurate Mass: 226.062995

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

Physical Description: Plates (EtOH)

Melting Point: Mp 200°

Other Data: Sublimes

Aldrich: B1240-7

Fluka: 12927

>>Derivative: Me ester

CAS Registry Number: 6158-54-9

Molecular Formula: C₁₅H₁₂O₃

Molecular Weight: 240.258

Accurate Mass: 240.078645

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

Physical Description: Cryst. (MeOH)

Melting Point: Mp 107°

Rare Chemicals Library: S14288-3

>>Derivative: Chloride

CAS Registry Number: 39148-58-8

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: Solid

Melting Point: Mp 98-99°

>>Derivative: Anilide

Synonym(s): 4-Benzoylbenzanilide

CAS Registry Number: 183235-14-5

Molecular Formula: C₂₀H₁₅NO₂

Molecular Weight: 301.344

Accurate Mass: 301.110279

Percentage Composition: C 79.72%; H 5.02%; N 4.65%; O 10.62%

Physical Description: Cryst. (toluene)

Melting Point: Mp 161-161.5°

>>Derivative: Nitrile

Synonym(s): 4-Cyanobenzophenone. 4-Benzoylbenzonitrile

CAS Registry Number: 1503-49-7

Molecular Formula: C₁₄H₉NO

Molecular Weight: 207.231

Accurate Mass: 207.068414

Percentage Composition: C 81.14%; H 4.38%; N 6.76%; O 7.72%

Melting Point: Mp 107-108°

Rare Chemicals Library: S87679-8

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 239B, (*ir*)

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

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

Wertheim, E., *J.A.C.S.*, 1933, **55**, 2541, (*synth*)

Kym, P.R. *et al.*, *J. Med. Chem.*, 1993, **36**, 1111, (*chloride*)

Perry, R.J. *et al.*, *J.O.C.*, 1996, **61**, 7482-7485, (*anilide, synth, pmr, cmr*)