



-->Entry Name: 4-Aminobenzophenone, (C)
Synonym(s): (4-Aminophenyl)phenylmethanone, (C)

CAS Registry Number: 1137-41-3

Molecular Formula: C₁₃H₉NO
Molecular Weight: 197.216
Accurate Mass: 197.084064
Percentage Composition: C 79.17%; H 5.62%; N 7.10%; O 8.11%
Physical Description: Leaflets (EtOH aq.)
Melting Point: Mp 124°
Boiling Point: Bp₁₁ 246°
Hazard & Toxicity: LD₅₀ (ma, ip) 300 mg/kg

Aldrich: A4140-2
Fluka: 7030
Sigma: A6887

-->Derivative: Oxime

Molecular Formula: C₁₃H₉N₂O
Molecular Weight: 212.251
Accurate Mass: 212.094963
Percentage Composition: C 73.57%; H 5.70%; N 13.20%; O 7.54%
Physical Description: Cryst. in two forms (EtOH or EtOH aq.)
Melting Point: Mp 126°, Mp 168°

-->Derivative: 2,6-Dinitrophenylhydrazone

Physical Description: Cryst.
Melting Point: Mp 189-191°

-->Derivative: N-Ac

CAS Registry Number: 6834-61-1
Molecular Formula: C₁₃H₉NO₃
Molecular Weight: 239.273
Accurate Mass: 239.094629
Percentage Composition: C 73.30%; H 5.48%; N 5.85%; O 13.37%
Physical Description: Needles (EtOH aq.)
Melting Point: Mp 156°

-->Derivative: N-Benzoyl

CAS Registry Number: 19617-84-6
Molecular Formula: C₁₃H₉NO₂
Molecular Weight: 201.244
Accurate Mass: 201.110279
Percentage Composition: C 79.72%; H 5.02%; N 4.65%; O 10.62%
Physical Description: Leaflets (EtOH)
Melting Point: Mp 152°

-->Derivative: N-Me

Synonym(s): 4-(Methylamino)benzophenone

CAS Registry Number: 26178-74-5
Molecular Formula: C₁₃H₁₁NO
Molecular Weight: 211.263
Accurate Mass: 211.099714
Percentage Composition: C 79.59%; H 6.20%; N 6.63%; O 7.57%
Physical Description: Yellow cryst. (petrol)
Melting Point: Mp 111° (82°)

-->Derivative: N,N-Di-Me

Synonym(s): 4-(Dimethylamino)benzophenone

CAS Registry Number: 530-44-9
Molecular Formula: C₁₃H₁₃NO
Molecular Weight: 225.29
Accurate Mass: 225.115564
Percentage Composition: C 79.97%; H 6.71%; N 6.22%; O 7.10%
Physical Description: Leaflets (EtOH)
Melting Point: Mp 92-93°
Aldrich: 14954-9

References:

Aldrich Library of 13C and 1H FT-NMR Spectra, 1992, 2, 900B, (nmr)
Aldrich Library of FT-IR Spectra, 1st edn, 1985, 2, 69A; 70A, (ir)
Aldrich Library of IR Spectra, 2nd Ed., 179D, (ir)
Aldrich Library of NMR Spectra, 6, 57C, (nmr)
Sadtler Standard C-13 NMR Spectra, 869Z, (nmr)
Sadtler Standard Ultraviolet Spectra, 5737, (uv)
Clark, L. et al., J.A.C.S., 1911, 33, 1135, (synth)
Heller, R. et al., Org. Mass Spectrom., 1974, 9, 1134, (ms)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, A1R250