



>>Entry Name: 3-Acetylbenzoic acid, 9CI
Synonym(s): Acetophenone-3-carboxylic acid

CAS Registry Number: 586-42-5

Molecular Formula: C₉H₈O₃
Molecular Weight: 164.16
Accurate Mass: 164.047345
Percentage Composition: C 65.85%; H 4.91%; O 29.24%
Physical Description: Cryst.
Melting Point: Mp 172° (166°)
pKa Value: pK_{a1} 3.83 (25°)

>>Derivative: Me ester

CAS Registry Number: 21860-07-1
Molecular Formula: C₁₀H₁₀O₃
Molecular Weight: 178.187
Accurate Mass: 178.062995
Percentage Composition: C 67.41%; H 5.66%; O 26.94%
Physical Description: Cryst. (Et₂O)
Melting Point: Mp 45-46°

>>Derivative: Ph ester

CAS Registry Number: 31076-87-6
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 75°

>>Derivative: Chloride

CAS Registry Number: 31076-85-4
Molecular Formula: C₉H₇ClO₂
Molecular Weight: 182.606
Accurate Mass: 182.013457
Percentage Composition: C 59.20%; H 3.86%; Cl 19.41%; O 17.52%
Physical Description: Liq.
Boiling Point: Bp_{0.4} 120°

>>Derivative: Nitrile

Synonym(s): 3'-Cyanoacetophenone

CAS Registry Number: 6136-68-1
Molecular Formula: C₉H₇NO
Molecular Weight: 145.16
Accurate Mass: 145.052764
Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%
Melting Point: Mp 98-100°
Aldrich: 29221-4

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1516B, (*nmr*)
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Rupe, H. *et al.*, *Ber.*, 1900, **33**, 3408, (*synth*)
Durif-Verambon, B. *et al.*, *Bull. Soc. Chim. Fr.*, 1970, 4452, (*synth*)
Exner, O. *et al.*, *Coll. Czech. Chem. Comm.*, 1971, **36**, 534, (*ir*)
Bromilow, J. *et al.*, *J.C.S. Perkin 2*, 1981, 753, (*cmr*)