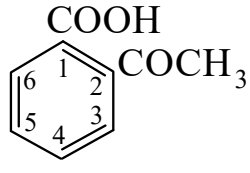
>>**Entry Name: 2-Acetylbenzoic acid,** 9CI
Synonym(s): Acetophenone-2-carboxylic acid



CAS Registry Number: 577-56-0

Molecular Formula: $C_9H_8O_3$
Molecular Weight: 164.16
Accurate Mass: 164.047345
Percentage Composition: C 65.85%; H 4.91%; O 29.24%
General Statement: Tautomeric with 3-Hydroxy-3-methyl-1(3*H*)-isobenzofuranone FCF19-Z
Physical Description: Cryst. (petrol)
Melting Point: Mp 117-118°
pKa Value: pK_{a1} 4.13 (25°)
Other Data: Exists as phthalide tautomer 3-Hydroxy-3-methyl-1(3*H*)-isobenzofuranone FCF19-Z in solid state and non-aq. soln., and as 2-acetylbenzoic acid only in aq. alkaline soln.

Aldrich: A1280-1
Fluka: 930

>>**Derivative:** Me ester

CAS Registry Number: 1077-79-8
Molecular Formula: $C_{10}H_{10}O_3$
Molecular Weight: 178.187
Accurate Mass: 178.062995
Percentage Composition: C 67.41%; H 5.66%; O 26.94%
Physical Description: Liq.
Boiling Point: Bp_2 94-95°

>>**Derivative:** Nitrile
Synonym(s): *o*-Cyanoacetophenone

CAS Registry Number: 91054-33-0
Molecular Formula: C_9H_7NO
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 39-42° (48°)

>>**Derivative:** Nitrile, phenylhydrazone

Melting Point: Mp 205-207°

References:

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