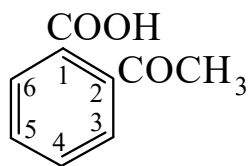




>>Entry Name: 2-Acetylbenzoic acid, 9CI
Synonym(s): Acetophenone-2-carboxylic acid



CAS Registry Number: 577-56-0

Molecular Formula: C₉H₈O₃

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: p*K*_{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: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Physical Description: Liq.

Boiling Point: Bp₂ 94-95°

>>Derivative: Nitrile

Synonym(s): *o*-Cyanoacetophenone

CAS Registry Number: 91054-33-0

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 39-42° (48°)

>>Derivative: Nitrile, phenylhydrazone

Melting Point: Mp 205-207°

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