



>>Entry Name: **3-Acetylbenzoic acid, 9Cl**

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°