



>>Entry Name: **4-Acetylbenzoic acid, 9CI**

Synonym(s): Acetophenone-4-carboxylic acid

CAS Registry Number: 586-89-0

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. (H₂O)

Melting Point: Mp 209-210°

pKa Value: pK_{a1} 3.7 (25°)

Aldrich: 17745-8

Fluka: 932

>>Derivative: Oxime (*E*-)

CAS Registry Number: 145578-44-5

Molecular Formula: C₉H₉NO₃

Molecular Weight: 179.175

Accurate Mass: 179.058244

Percentage Composition: C 60.33%; H 5.06%; N 7.82%; O 26.79%

Melting Point: Mp 215-216°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange needles (AcOH)

Melting Point: Mp 280 dec.°

>>Derivative: Me ester

CAS Registry Number: 3609-53-8

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

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

Physical Description: Needles (C₆H₆/hexane), plates (CCl₄ or hexane)

Melting Point: Mp 95-95.5°