



>>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°

>>Derivative: Et ester

CAS Registry Number: 38430-55-6
Molecular Formula: C₁₁H₁₂O₃
Molecular Weight: 192.214
Accurate Mass: 192.078645
Percentage Composition: C 68.74%; H 6.29%; O 24.97%
Physical Description: Needles (H₂O)
Melting Point: Mp 55-57°

>>Derivative: Ph ester

CAS Registry Number: 31076-86-5
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. (EtOH)
Melting Point: Mp 122°