



>>Entry Name: 5-Acetyl-2-hydroxybenzoic acid

Synonym(s): 3'-Carboxy-4'-hydroxyacetophenone. 5-Acetylsalicylic acid

CAS Registry Number: 13110-96-8

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Needles (EtOH)

Melting Point: Mp 215-216°

Rare Chemicals Library: S38695-2

>>Derivative: Me ester

CAS Registry Number: 16475-90-4

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Physical Description: Prisms (MeOH)

Melting Point: Mp 62°

Aldrich: 39020-8

>>Derivative: Amide

CAS Registry Number: 40187-51-7

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%

Physical Description: Cryst.

Melting Point: Mp 220-222°

>>Derivative: Me ether

Synonym(s): 5-Acetyl-2-methoxybenzoic acid. 3'-Carboxy-4'-methoxyacetophenone

CAS Registry Number: 68535-61-5

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Melting Point: Mp 137°

References:

Granger, R. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1952, **234**, 1058, (*synth, amide*)

Jones, H. *et al.*, *J. Med. Chem.*, 1978, **21**, 1100, (*synth, deriv*)

Leclerc, G. *et al.*, *J. Med. Chem.*, 1980, **23**, 738, (*synth*)