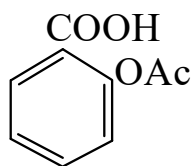




>>Entry Name: **2-Acetoxybenzoic acid**

Synonym(s): 2-Acetyloxybenzoic acid, 9CI. Salicylic acid acetate, 8CI. Acetylsalicylic acid. **Aspirin**, BAN, USAN



CAS Registry Number: 50-78-2

Related CAS Registry Numbers(s): 493-53-8 5749-67-7 37933-78-1

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

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

Biological Source: Constit. of *Glycyrrhiza glabra* var. *typica* roots. Produced industrially by acetylation of 2-Hydroxybenzoic acid [BLP36-T](#) with Acetic anhydride [DFR94-Z](#)

Use/Importance: Used as soln. in 10% ammonia for photometric detn. of Mn ($\lambda_{\max}$ 385 nm; in the presence of H₂O₂)

Biological Use/Importance: Analgesic, antipyretic and antiinflammatory agent.

Physical Description: Cryst.

Melting Point: Mp 135° (rapid heat). Fp 118°

pKa Value: pK_a 3.38 (25°, 1M KCl)

Calculated Log P Data: Log P 1.02 (calc)

Other Data: Ca salt used in combination with urea as Carbaspirin calcium, USAN

Hazard & Toxicity: Dust explosion haz. Irritant. Main adverse effects are gastrointestinal, with other dose dependent systemic effects. LD₅₀ (rat, orl) 200 mg/kg. Exp. teratogenic effects. OES: long-term 5 mg m⁻³

Aldrich: 13292-6

Fluka: 1459

Sigma: A5376

>>Derivative: Me ester

CAS Registry Number: 580-02-9

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Physical Description: Cryst. (petrol)

Melting Point: Mp 49°

Rare Chemicals Library: S43305-5

>>Derivative: Et ester

CAS Registry Number: 529-68-0

Molecular Formula: C₁₁H₁₂O₄

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Physical Description: Liq.

Boiling Point: Bp 289°. Bp 272°

Rare Chemicals Library: S39167-0

>>Derivative: Propyl ester

CAS Registry Number: 60310-03-4

Molecular Formula: C₁₂H₁₄O₄

Molecular Weight: 222.24

Accurate Mass: 222.08921

Percentage Composition: C 64.85%; H 6.35%; O 28.80%

Physical Description: Light yellow liq.

Boiling Point: Bp 289°. Bp₁₀ 162-164°