



>>Entry Name: Benzoic acid, 9CI, USAN

ENTRY UNDER REVIEW

Synonym(s): Benzenecarboxylic acid. E 210. FEMA 2131

CAS Registry Number: 65-85-0

Related CAS Registry Numbers(s): 766-76-7 1079-02-3 8000-95-1 43019-90-5

PhCOOH

Molecular Formula: C₇H₆O₂

Molecular Weight: 122.123

Accurate Mass: 122.03678

Percentage Composition: C 68.85%; H 4.95%; O 26.20%

General Statement: For salts see Benzoic acid salts [GOG67-I](#)

Biological Source: Widespread in plants esp. in essential oils, mostly in esterified form. Obt. in 17th Century by sublimation of *Styrax* spp. resin. Produced industrially mainly by oxidation of toluene

Use/Importance: Preservative in the food industry. Used in manuf. of preservatives, plasticisers, alkyd resin coatings and caprolactam. Antiseptic, expectorant, antifungal, antipyretic, keratolytic agent. Used as alkalimetric standard; in photometric detn. of U and Zr (anionic complexes associated with basic dyes). Reference material used in elemental microanalysis

Physical Description: Leaflets or needles (H₂O)

Melting Point: Mp 122°

Boiling Point: Bp 249°. Bp₁₀ 133°

Solubility: V. spar. sol. H₂O; BERDY SOL: Sol. MeOH, C₆H₆; fairly sol. hexane; poorly sol. H₂O

Calculated Log P Data: Log P 1.88 (calc)

UV: [neutral] λ_{max} 228 (E1%/1cm 728); 273 (E1%/1cm 93.2); 300 (E1%/1cm 46.8) (MeOH) (Berdy)

Other Data: Steam-volatile

Hazard & Toxicity: Fl. p. 121°, autoignition temp. 570°. Eye, skin and mucous membrane irritant. Hypersensitivity reactions reported. Low systemic toxicity

Aldrich: W21312-8

Fluka: 12350

Sigma: B3250

Supelco: R43-2000

>>Derivative: Me ester

Synonym(s): Methyl benzoate. FEMA 2683

CAS Registry Number: 93-58-3

Molecular Formula: C₈H₈O₂

Molecular Weight: 136.15

Accurate Mass: 136.05243

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Biological Source: Present in various flower oils and fruits

Use/Importance: Used in perfumery and flavourings

Physical Description: Liq. with fruity odour

Melting Point: Fp -12.3°

Boiling Point: Bp 199.6°. Bp₂₄ 96-98°

Density: d₂₅²⁵ 1.09

Hazard & Toxicity: Fl. p. 83°. Skin and eye irritant. LD₅₀ (rat, orl) 1350 mg/kg

Aldrich: M2990-8

Fluka: 12460

Sigma: B0893

>>Derivative: Et ester

Synonym(s): Ethyl benzoate. FEMA 2422

CAS Registry Number: 93-89-0

Molecular Formula: C₉H₁₀O₂

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Biological Source: Found in various fruits, e.g. apple, banana

Use/Importance: Polymerisation catalyst. Used in perfumery and flavourings

Physical Description: Liq. with aromatic/fruity odour

Melting Point: Fp -34°

Boiling Point: Bp 212.9°. Bp₁₀ 87.2°

Density: d