>>**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: $C_7H_6O_2$
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 (H_2O)
Melting Point: Mp 122°
Boiling Point: Bp 249°. Bp_{10} 133°
Solubility: V. spar. sol. H_2O; BERDY SOL: Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O
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: $C_8H_8O_2$
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°. Bp_{24} 96-98°
Density: d_{25}^{25} 1.09
Hazard & Toxicity: Fl. p. 83°. Skin and eye irritant. LD_{50} (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: $C_9H_{10}O_2$
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°. Bp_{10} 87.2°
Density: d