



>>Entry Name: Benzaldehyde, USAN

ENTRY UNDER REVIEW

Synonym(s): Benzenecarboxaldehyde. Formylbenzene. FEMA 2127

CAS Registry Number: 100-52-7

Related CAS Registry Numbers(s): 932-90-1 3592-47-0

PhCHO

Molecular Formula: C₇H₆O

Molecular Weight: 106.124

Accurate Mass: 106.041865

Percentage Composition: C 79.23%; H 5.70%; O 15.08%

Biological Source: Found in plants, esp. in almond kernels and those of other prunes spp. Also present in strawberry jam, leek, crispbread, cheese, black tea and several essential oils

Use/Importance: Parent and derivs. (e.g. glyceryl acetal) are used as flavourings. Used for photometric detn. of O₃. Forms benzylidene derivs. with sugars for characterisation, OH group protection and for use in ms analysis. Forms Schiff's bases with amines.

Biological Use/Importance: Shows antispasmodic, anaesthetic and antineoplastic props.

Physical Description: Liq. with characteristic almond-type odour

Melting Point: Mp -26°. Fp -56.9°

Boiling Point: Bp 178-179°. Bp₁₀ 62°

Solubility: V. spar. sol. H₂O; misc. org. solvs.

Density: d₄¹⁵ 1.0504

pKa Value: pK_a 14.9 (25°,hydrate, 1% EtOH) pK_a -6.9 (as base)

Calculated Log P Data: Log P 1.5 (calc)

UV: [neutral] λ_{max} 244 (); 280 () (MeOH) (Berdy)

Other Data: Steam-volatile. Forms bisulfite compd. Slowly oxid. in air. Reduces AgNO₃.NH₂ but not Fehling's soln.

Hazard & Toxicity: Fl. p. 63°, autoignition temp. 190°. Violently oxid. by 90% HCOOOH. Skin irritant. May cause dermatitis. CNS depressant. LD₅₀ (rat, orl) 1300 mg/kg

Aldrich: W21270-9

Fluka: 12015

Sigma: B6259

Supelco: 48-2127

>>Derivative: (E)-Oxime

Synonym(s): α-Benzaldoxime

CAS Registry Number: 622-31-1

Molecular Formula: C₇H₇NO

Molecular Weight: 121.138

Accurate Mass: 121.052764

Percentage Composition: C 69.41%; H 5.82%; N 11.56%; O 13.21%

Use/Importance: Used as EtOH soln. for detn. of Co and Ni (pptn.)

Physical Description: Needles

Melting Point: Mp 35°

Boiling Point: Bp₁₀ 118-119°

Solubility: Sol. EtOH

>>Derivative: (Z)-Oxime

Synonym(s): β-Benzaldoxime

CAS Registry Number: 622-32-2

Molecular Formula: C₇H₇NO

Molecular Weight: 121.138

Accurate Mass: 121.052764

Percentage Composition: C 69.41%; H 5.82%; N 11.56%; O 13.21%

Physical Description: Needles (Et₂O)

Melting Point: Mp 130°

Other Data: Gradually inverts to (E)-form, more rapidly on heating or by dil. acids

Aldrich: 24567-4