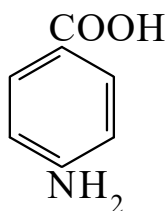




>>Entry Name: 4-Aminobenzoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Vitamin H'. Aminobenzoic acid, USAN. PABA



CAS Registry Number: 150-13-0

Related CAS Registry Numbers(s): 138-84-1 515-74-2 555-06-6 577-48-0 64059-66-1 75106-10-4

Extra CAS Registry Numbers(s): 1321-11-5

Molecular Formula: $C_7H_7NO_2$

Molecular Weight: 137.138

Accurate Mass: 137.047679

Percentage Composition: C 61.31%; H 5.14%; N 10.21%; O 23.33%

Source/Synthesis: Manuf. by redn. of 4-nitrobenzoic acid

Biological Source: Prod. by yeasts and bacteria

Use/Importance: Reagent for characterisation of aldoses. Used as a growth factor, an antirickettsial and as a sunscreen agent. Bacterial growth factor. Used as 1.5% soln. in 0.1M NaOH for gravimetric detn. of Cu(II). Monomer for polyamide fibres

Physical Description: Prisms

Melting Point: Mp 188-188.5°

Solubility: Sol. H_2O , alkalis, EtOH, Et_2O , C_6H_6

pKa Value: pK_{a1} 2.5; pK_{a2} 4.87 (25°)

Calculated Log P Data: Log P 0.98 (calc)

Other Data: Discolours to orange on exp. to air and light

Hazard & Toxicity: Can cause contact and photocontact allergic dermatitis from topical use. LD_{50} (rbt, orl) 1830 mg/kg. Exp. reprod. effects

Aldrich: 10053-6

Fluka: 6940

Sigma: A9878

Supelco: R47-2625

>>Derivative: Me ester

Synonym(s): Methyl 4-aminobenzoate

CAS Registry Number: 619-45-4

Molecular Formula: $C_8H_9NO_2$

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 112°

Aldrich: 27418-6

Fluka: 6990