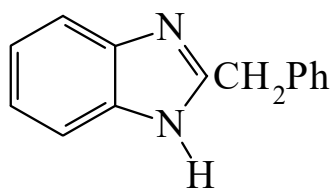




>>Entry Name: 2-Benzylbenzimidazole, 8CI

Synonym(s): 2-(Phenylmethyl)-1*H*-benzimidazole, 9CI. Bendazol, INN



CAS Registry Number: 621-72-7

Molecular Formula: C₁₄H₁₂N₂

Molecular Weight: 208.262

Accurate Mass: 208.100048

Percentage Composition: C 80.74%; H 5.81%; N 13.45%

Use/Importance: Coronary vasodilator, spasmolytic, antihypertensive agent

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 187°

Solubility: BERDY SOL: Sol. MeOH, Et₂O, H₂O; fairly sol. C₆H₆; poorly sol. hexane

pKa Value: pK_a 5.7

Calculated Log P Data: Log P 3.63 (calc)

UV: [neutral] λ_{max} 276 (E1%/1cm 685) (MeOH) (Berdy) [neutral] λ_{max} (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 100 mg/kg. Exp. reprod. and teratogenic effects ; BERDY HAZD : LD₅₀ (mus, ivn) 25 - 35 mg/kg , LD₅₀ (mus, scu) 15 mg/kg , LD₅₀ (mus, orl) 35 mg/kg

Rare Chemicals Library: S35825-8

>>Derivative: Hydrochloride

Synonym(s): Dibazol. Tromasedan

Physical Description: Greyish or yellow-white hygroscopic powder with bitter-saline taste

Melting Point: Mp 175°

Solubility: Insol. Et₂O; v. sol. hot H₂O

>>Derivative: 1-Me

Molecular Formula: C₁₅H₁₄N₂

Molecular Weight: 222.289

Accurate Mass: 222.115698

Percentage Composition: C 81.05%; H 6.35%; N 12.60%

Physical Description: Pale pink cryst. (cyclohexane)

Melting Point: Mp 72°

References:

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