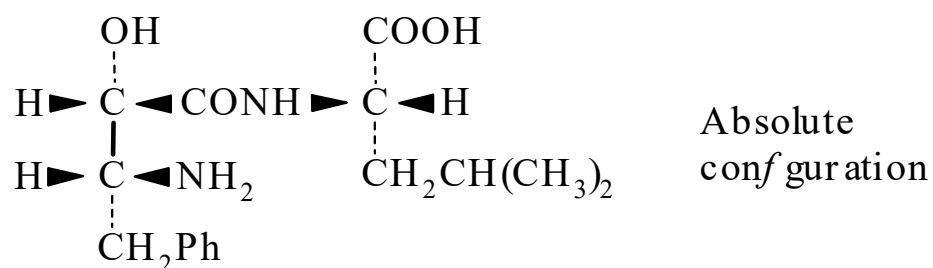




>>Entry Name: Bestatin

Synonym(s): *N*-(3-Amino-2-hydroxy-1-oxo-4-phenylbutyl)leucine, 9Cl. **Ubenimex**, INN. Inobestin. NK 421



CAS Registry Number: 58970-76-6

Related CAS Registry Numbers(s): 65391-42-6 100992-60-7

Molecular Formula: C₁₆H₂₄N₂O₄

Molecular Weight: 308.377

Accurate Mass: 308.173608

Percentage Composition: C 62.32%; H 7.84%; N 9.08%; O 20.75%

General Statement: Peptide antibiotic

Biological Source: Prod. by *Streptomyces olivoreticuli*

Use/Importance: Inhibitor of aminopeptidase B. Shows antineoplastic props. with clinical potential. Immunomodulator

Physical Description: Needles

Development Status: Launched 1987

Melting Point: Mp 233-236°

Optical Rotation: $[\alpha]_D^{20} -15.5$ (c, 1 in 1M HCl)

Solubility: BERDY SOL: Sol. MeOH, DMSO, AcOH; fairly sol. H₂O; poorly sol. EtOAc, hexane, C₆H₆, CHCl₃

Calculated Log P Data: Log P -0.48 (calc)

UV: [neutral] $\lambda_{\max}$ 248 (ε 104); 253 (ε 139); 259 (ε 172); 265 (ε 132); 268 (sh) (ε 75) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 248 (ε 104); 253 (ε 130); 258 (ε 172); 264 (ε 132) (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 241 (); 248 (); 253 (); 258 (); 264 (); 268 () (H₂O) (Berdy)

Hazard & Toxicity: LD₅₀ (rat, ipr) 780 mg/kg. Exp. reprod. effects (v. large dose) ; BERDY HAZD : LD₅₀ (mus, ipr) 300 - 700 mg/kg

Sigma: B9274

References:

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