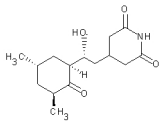

Formula: C15H23NO4

MW: 281.35

CAS: 66-81-9

TNP NUMBER: TNP00309

MDL NUMBER: MFCD02114267

IUPAC: 4-[(2R)-2-((1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl]azaperhydro ine-2,6-dione

Smiles: C([C@@H](O)[C@H]1(C(=O)[C@@H](C)C[C@@H](C1)C))C1CC(=O)NC(C1)=O

ACCEPTORS: 4

DONORS: 2

ROTATION BONDS: 3

N+O: 5

Chiral Centers: 4

LogP: 0.2

LogS: -3.2

LIPINSKI: 4

Monograph Number: 0002757

Title: Cycloheximide

CAS Registry Number: 66-81-9

CAS Name:
[1S-[1a(S*),3a,5b]]-4-[2-(3,5-Dimethyl-2-oxocyclohexyl)-2-hydroxyethyl]-2,6-piperidinedione

Additional Names: 3-[2-(3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl]glutarimide; naramycin A

Manufacturers' Codes: NSC-185; U-4527

Trademarks: Actidione (Upjohn)

Molecular Formula: C15H23NO4

Molecular Weight: 281.35.

Percent Composition: C 64.03%, H 8.24%, N 4.98%, O 22.75%

Literature References: Antibiotic substance isolated from the beers of streptomycin-producing strains of Streptomyces griseus: B. E. Leach et al., J. Am. Chem. Soc. 69, 474 (1947); J. H. Ford, B. E. Leach, ibid. 70, 1223 (1948); A. J. Whiffen et al., US 2574519 (1951 to Upjohn). Production, assay and antibiotic activity: A. J. Whiffen, J. Bacteriol. 56, 283 (1948). Improved production method: Kominek, US 3915802; US 3915803 (both 1975 to Upjohn). Structure: E. C. Kornfeld et al., J. Am. Chem. Soc. 71, 150 (1949). Absolute configuration: E. J. Eisenbraun et al., ibid. 80, 1261 (1958); F. Johnson, N. A. Starkovsky, Tetrahedron Lett. 1962, 1173; F. Johnson et al., J. Am. Chem. Soc. 87, 4612 (1965). Synthesis of dl- and l-forms: F. Johnson et al., ibid. 88, 149 (1966).

Properties: Plates from amyl acetate or water or 30% methanol, mp 119.5-121 (Whiffen, 1951); also reported as mp 115-116 (Johnson, 1966). [a]D29 -3.38 (c = 9.47 in methanol); [a]D25 +6.8 (c = 2 in H2O). Soly at 2: water 2.1 g/100 ml, amyl acetate 7 g/100 ml. Also sol in chloroform, ether, acetone, methanol, ethanol, other common organic solvents except satd hydrocarbons. Relatively heat-stable, acid-stable, destroyed by boiling in aq soln at pH 7 for 1 hr, but shows no loss of activity after 15 min boiling. At pH 2 it is not destroyed by boiling for 1 hr. Rapidly inactivated at room temp by dil alkali with the formation of a volatile, fragrant ketone, 2,4-dimethylcyclohexanone. Extremely repellent to rats. LD50 i.v. in mice: 150 mg/kg (Leach).

Melting point: mp 119.5-121 (Whiffen, 1951); mp 115-116 (Johnson, 1966)

Optical Rotation: [a]D29 -3.38 (c = 9.47 in methanol); [a]D25 +6.8 (c = 2 in H2O)

Toxicity data: LD50 i.v. in mice: 150 mg/kg (Leach)

Derivative Type: Acetate

Molecular Formula: C17H25NO5

Molecular Weight: 323.38.

Percent Composition: C 63.14%, H 7.79%, N 4.33%, O 24.74%

Properties: Glistening plates from methanol, mp 148-149. [a]D25 +22 (c = 2.3 in methanol).

Melting point: mp 148-149

Optical Rotation: [a]D25 +22 (c = 2.3 in methanol)

Use: Fungicide; plant growth regulator. As protein synthesis inhibitor.

Synonyms: LEGIONELLA COMBI PACK;Cycloheximide liquor;((dimethyl-3,5oxo-2cyclohexyl)-2hydroxy-2ethyl)-3glutarimide;[1s-[1alpha(s*),3alpha,5beta]]-4-[2-(3,5-dimethyl-2-oxo-cyclohexyl)]-2-hydroxy;3-(2-(3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl)-glutarimid;3alpha,5beta))-(1alpha(s*;5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl)-6-piperidinedion(1s-4-(2-(3;Actidionebr

CAS:66-81-9

MF:C15H23NO4

MW:281.34742

EINECS:200-636-0

Product Categories:Miscellaneous;Antibiotic Explorer;Antifungal;Signalling;Antibiotics Actidione

Chemical Properties: mp 111-116 C alpha -28.5 (c=1, CHCl3) storage temp. 2-8C Water Solubility 2.1 g/100 mL (2 C) Stability:Stable. Combustible. Incompatible with strong oxidizing agents, acid chlorides, acid anhydrides, alkali.

CAS DataBase Reference: 66-81-9(

CAS DataBase Reference:) EPA Substance Registry System2,6-Piperidinedione, 4-[(2R)-2-[(1S,3S,5S)-3,5- dimethyl-2-oxocyclohexyl]- 2-hydroxyethyl]-(66-81-9) Xn,T,N,T+ Risk Statements 22-68-61-51/53-28 Safety Statements 53-45-61 RIDADR UN 2811 6.1/PG 1 WGK Germany 3 RTECS MA4375000 HazardClass 6.1(a) PackingGroup II Hazardous Substances Data66-81-9(Hazardous Substances Data) Actidione

Usage And Synthesis:

Chemical Properties: Off-white to light tan powder General DescriptionColorless crystals. Used as a fungicide and as a anticancer drug. Air & Water ReactionsWater soluble. Reactivity ProfileActidione is an imide. Actidione is incompatible with strong oxidizing agents, acid chlorides and acid anhydrides. Actidione decomposes rapidly in alkali at room temperature. Health HazardActidione is extremely toxic; the probable oral lethal dose in humans is 5-50 mg/kg, or 7 drops to 1 teaspoonful for a 150-lb. person. Fire HazardWhen exposed to heat, Actidione emits toxic fumes, including nitrogen oxides. Biological ActivitySelective inhibitor of eukaryotic (over prokaryotic) protein synthesis, blocking tRNA binding and release from ribosomes. Induces apoptosis in a variety of transformed and normal cell lines, including T-cells. Competitively inhibits the PPIase hFKBP12 (K i = 3.4 u M). Antifungal antibiotic. Actidione