



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]azaperhydroine-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). $[\alpha]_{D29} -3.38$ (c = 9.47 in methanol); $[\alpha]_{D25} +6.8$ (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: $[\alpha]_{D29} -3.38$ (c = 9.47 in methanol); $[\alpha]_{D25} +6.8$ (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. $[\alpha]_{D25} +22$ (c = 2.3 in methanol).

Melting point: mp 148-149

Optical Rotation: $[\alpha]_{D25} +22$ (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 System 2,6-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 Data 66-81-9 (Hazardous Substances Data) Actidione

Usage And Synthesis:

Chemical Properties: Off-white to light tan powder General Description Colorless crystals. Used as a fungicide and as an anticancer drug. Air & Water Reactions Water soluble. Reactivity Profile Actidione is an imide. Actidione is incompatible with strong oxidizing agents, acid chlorides and acid anhydrides. Actidione decomposes rapidly in alkali at room temperature. Health Hazard Actidione 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 Hazard When exposed to heat, Actidione emits toxic fumes, including nitrogen oxides. Biological Activity Selective 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 ($K_i = 3.4 \mu\text{M}$). Antifungal antibiotic. Actidione

