ST056390 Colchicine

Formula: C22H25NO6

MW: 399.44

CAS: 64-86-8

TNP NUMBER: TNP00005

MDL NUMBER: MFCD00001179

IUPAC: N-((7S)-1,2,3,10-tetramethoxy-9-oxo-5,6,7-trihydrobenzo[d]heptalen-7-yl)acetamide

Smiles: c12c(cc(=O)c(cc2)OC)C(NC(=O)C)CCc2c1c(c(OC)c(c2)OC)OC

THERAPEUTIC CATEGORY: Gout suppressant. Treatment of Familial Mediterranean Fever

VET THERAP CATEGORY: Antineoplastic

Colchicine


SOURCE: A major alkaloid of Colchicum autumnale L., Liliaceae

ACCEPTORS: 6

DONORS: 1

ROTATION BONDS: 4

N+O: 7

Chiral Centers: 1

LogP: 3.06

LogS: -4.61

LIPINSKI: 4

Monograph Number: 0002496

Title: Colchicine

CAS Registry Number: 64-86-8

CAS Name: N-[(7S)-5,6,7,9-Tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo[a]heptalen-7-yl]acetamide

Molecular Formula: C22H25NO6

Molecular Weight: 399.44.

Percent Composition: C 66.15%, H 6.31%, N 3.51%, O 24.03%


Properties: Pale yellow scales or powder, mp 142-150. Darkens on exposure to light. Has been crystallized from ethyl acetate, pale yellow needles, mp 157. [a]D17 -429 (c = 1.72). [a]D17 -121 (c = 0.9 in chloroform). pK at 20: 12.35; pH of 0.5% soln: 5.9. uv max (95% ethanol): 350.5, 243 nm (log e 4.22; 4.47). One gram dissolves in 22 ml water, 220 ml ether, 100 ml benzene; freely sol in alcohol or chloroform. Practically insol in petr ether. Forms two cryst compds with chloroform, B.CHCl3 or B.2CHCl3, which do not give up their chloroform unless heated between 60 and 70 for considerable time. LD50 in rats (mg/kg): 1.6 i.v. (Rosenbloom, Ferguson); in mice (mg/kg): 4.13 i.v. (Beliles).

Melting point: mp 142-150; mp 157

pKa: pK at 20: 12.35; pH of 0.5% soln: 5.9

Optical Rotation: [a]D17 -429 (c = 1.72); [a]D17 -121 (c = 0.9 in chloroform)

Absorption maximum: uv max (95% ethanol): 350.5, 243 nm (log e 4.22; 4.47)

Toxicity data: LD50 in rats (mg/kg): 1.6 i.v. (Rosenbloom, Ferguson); in mice (mg/kg): 4.13 i.v. (Beliles)

Use: In research in plant genetics (for doubling chromosomes).

Therap-Cat: Gout suppressant. Treatment of Familial Mediterranean Fever.

Therap-Cat-Vet: Has been used as an antineoplastic.

Synonyms:
(S)-N-(5,6,7,9-TETRAHYDRO-1,2,3,10-TETRAMETHOXY-9-OXOGENZO[A]HEPTALEN-7-YL) ACETAMIDE;N-((S)-1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRAHYDRO-BENZO[A]HEPTALEN-7-YL)-ACETAMIDE;n-(5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenz[a]heptalen-7-yl)-acetamide;7-acetamido-6,7-dihydro-1,2,3,10-tetramethoxy-benzo(a)heptalen-9(5h)-on;7-alpha-h-colchicine;7alpha-h-colchicine;7alphaH-Colchicine;Acetamide, N-(5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenz[a]heptalen-7-yl)-
ST056390 Colchicine

CAS: 64-86-8

MF: C22H25NO6

MW: 399.44

EINECS: 200-598-5

Product Categories: Alkaloids; All Inhibitors; Alkaloids (Others); Biochemistry; Plant Growth Regulators; Plant Growth Triggers (Others); Tropolones; Tropolones & Azulenes; Antibiotic Explorer; Inhibitors; Intermediates & Fine Chemicals; Pharmaceuticals; API's; Antitumor Agents; Cell Signaling and Neuroscience; Cytoskeleton and Extracellular Matrix; Microtubule Inhibitors; Cancer Research; Microtubule Inhibitors; Caspases/Apoptosis

Chemical Properties: mp 150-160 °C (dec.)(lit.) alpha -250° (c=1, alcohol) storage temp. Poison room solubility H2O: 10 mg/mL form powder color white to yellow with a green cast Water Solubility 45 g/L (20 C) Sensitive Light Sensitive Merck 14,2471 BRN 2228813 Stability: Stable. Light sensitive. Incompatible with strong oxidizing agents.

CAS DataBase Reference: 64-86-8

Usage And Synthesis:

Chemical Properties: Yellow Solid Usage An antimitotic agent that disrupts microtubules by binding to tubulin and preventing its polymerization. Stimulates the intrinsic GTPase activity of tubulin. Induces apoptosis in several normal and tumor cell lines and activates the JNK/SAPK signal General Description Odorless or nearly odorless pale yellow needles or powder that darkens on exposure to light. Used to treat gouty arthritis, pseudogout, sarcoidal arthritis and calcific tendinitis. Air & Water Reactions Slowly hydrolyzed in acidic solution, but unbuffered solutions are stable at 68F for at least six months. Isomerizes on exposure to ultraviolet radiation. Reactivity Profile Colchicine darkens on exposure to light. Incompatible with strong oxidizing agents. Also incompatible with mineral acids. Health Hazard Colchicine is classified as super toxic. Probable oral lethal dose in humans is less than 5 mg/kg, i.e. less than 7 drops for a 70 kg (150 lb.) person. Death results from respiratory arrest. The fatal dose varies considerably; as little as 7 mg of Colchicine has proved fatal. Fire Hazard Stable. Biological Activity Plant-derived alkaloid that binds to tubulin and depolymerizes microtubules. Colchicine