



Formula: C₂₃H₂₂O₆

MW: 394.42

CAS: 83-79-4

TNP NUMBER: TNP00301

MDL NUMBER: MFCD00599610

IUPAC: (12a*S*,6a*S*,2*R*)-8,9-dimethoxy-2-(1-methylvinyl)-1,2-dihydrochromano[3,4-*b*]furano[2,3-*h*]chroman-6-one

Smiles:

C([C@@H]1Oc2c(c3O[C@H]4[C@@H](C(=O)c3cc2)c2c(OC4)cc(c(c2)OC)OC)C1)(=C)C

VET THERAP CATEGORY: Ectoparasitic

Pesticide

REFERENCE: Merck 13,8350

SOURCE: Principal insecticidal constituent of derris root, cube, etc. Isolation from *Lonchocarpus nicou* (aubl.) DC., Leguminosae.

ACCEPTORS: 6

DONORS: 0

ROTATION BONDS: 2

N+O: 6

Chiral Centers: 3

LogP: 4.51

LogS: -5.1

LIPINSKI: 4

Synonyms: (-)-cis-rotenone;(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6alphaH)-one, 1,2,12,12alpha-tetrahydro-2alpha-isopropenyl-8,9-dimethoxy-;(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6aH)-one, 1,2,12,12a-tetrahydro-2-alpha-iospropenyl-8,9-dimethoxy-;(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6aH)-one, 1,2,12,12a-tetrahydro-2-alpha-isopropenyl-8,9-dimethoxy-;(1)benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6alphah)-one, 1,2,12,12alpha-t-(2r-(2alpha,6alpha,12alpha))-9-dimethoxy-2-(1-methylethenyl)-;(2R,2alpha,6alpha,12alpha)-1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)[1]benzopyrano[3,4-b]furo[2,3-H][1]benzopyran-6(6aH)-one;[1]Benzopyrano[3,4-b]furo[2,3-h][1]benzopyran-6(6aH)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, [2R-(2alpha,6alpha,12alpha)]-

CAS:83-79-4

MF:C23H22O6

MW:394.42

EINECS:201-501-9

Product Categories:Miscellaneous Natural Products;Alpha sort;BotanicalsPesticides&Metabolites;Q-ZAnalytical Standards;BotanicalsAnalytical Standards;Alphabetic;Insecticides;Pesticides;R;Mitochondrial Inhibitors;Cell Stress;Nitric Oxide and Cell Stress;Asymmetric Synthesis;Chiral Building Blocks;Complex Molecules ROTENONE

Chemical Properties: mp 159-164 C(lit.) bp 210-220 C0.5 mm Hg(lit.) alpha -115 (C=1.4 IN CHLOROFORM) storage temp. Store at RT Merck 13,8350 Stability:Stable, but light and air sensitive. Combustible. Incompatible with oxidizing agents, especially in the presence of alkalis. NIST Chemistry ReferenceRotenone(83-79-4) EPA Substance Registry System[1]Benzopyrano[3, 4-b]furo[2,3-h][1]benzopyran- 6(6aH)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, (2R,6aS,12aS)-(83-79-4) T,N Risk Statements 25-36/37/38-50/53 Safety Statements 22-24/25-36-45-60-61 RIDADR UN 2811 6.1/PG 3 WGK Germany 3 RTECS DJ2800000 HazardClass 6.1(b) PackingGroup III Hazardous Substances Data83-79-4(Hazardous Substances Data) ROTENONE

Usage And Synthesis:

Chemical Properties: white or off-white powder General Description Colorless to brownish crystals or a white to brownish-white crystalline powder. Has neither odor nor taste. Air & Water Reactions ROTENONE decomposes upon exposure to light or air. Insoluble in water. Reactivity Profile ROTENONE is readily oxidized in the presence of alkalis. ROTENONE is incompatible with oxidizers. Fire Hazard Flash point data for ROTENONE are not available; however, ROTENONE is probably combustible. Biological Activity Mitochondrial electron transport chain inhibitor (IC 50 = 1.7 - 2.2 μ M at complex I). Inhibits NADH oxidation by cardiac sarcoplasmic reticulum (IC 50 = 3.4 nM). Commonly used pesticide and induces Parkinsonism in animal models. Cell-permeable and brain penetrant. ROTENONE

