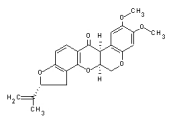

Formula: C23H22O6

MW: 394.42

CAS: 83-79-4

TNP NUMBER: TNP00301

MDL NUMBER: MFCD00599610

IUPAC: (12aS,6aS,2R)-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: Ectoparasistic

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(6aalphaH)-one, 1,2,12,12aalpha-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,1,2,12,12aalpha-t;(2r-(2alpha,6aalpha,12aalpha))--9-dimethoxy-2-(1-methylethenyl)-;(2R,2alpha,6aalpha,12aalpha)-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,6aalpha,12aalpha)]-

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 alkalies. 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 DescriptionColorless to brownish crystals or a white to brownish-white crystalline powder. Has neither odor nor taste. Air & Water ReactionsROTENONE decomposes upon exposure to light or air. Insoluble in water. Reactivity ProfileROTENONE is readily oxidized in the presence of alkalis. ROTENONE is incompatible with oxidizers. . Fire HazardFlash point data for ROTENONE are not available; however, ROTENONE is probably combustible. Biological ActivityMitochondrial electron transport chain inhibitor (IC 50 = 1.7 - 2.2 u 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