



Formula: C₁₀H₁₂O₄

MW: 196.2

CAS: 56-25-7

TNP NUMBER: TNP00289

MDL NUMBER: MFCD00044767

IUPAC: 2,6-dimethyl-4,10-dioxatricyclo[5.2.1.0]decane-3,5-dione

Smiles: CC12C(C)(C3OC1CC3)C(OC2=O)=O

Active principle of cantharides and other insects, in notorious 'spanish fly' aphrodisiac

THERAPEUTIC CATEGORY: Vesicant

VET THERAP CATEGORY: Rubifacient, Vesicant, Counterirritant

REFERENCE: Knapp, et al., The protein phosphatase inhibitor cantharidin alters vascular endothelial cell permeability. J. Pharmacol. Exp. Ther. 289, 1480-1486, (1999) abstract
Krieser, et al., Cleavage and nuclear translocation of the caspase 3 substrate Rho GDP-dissociation inhibitor, D4-GDI, during apoptosis. Cell Death Differ. 6, 412-419, (1999) abstract
Baskin, T.I., and Wilson J.E., Inhibitors of protein kinases and phosphatases alter root morphology and disorganize cortical microtubules. Plant Physiol. 113, 493-502, (1997) abstract
Knapp, et al., Contractility and inhibition of protein phosphatases by cantharidin. Gen. Pharmacol. 31, 729-733, (1998) abstract Merck Merck 13,1757

ACCEPTORS: 4

DONORS: 0

ROTATION BONDS: 0

N+O: 4

Chiral Centers: 4

LogP: 0.19

LogS: -2.85

LIPINSKI: 4

Synonyms: (1r,2s,3r,6s)-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboxylic anhydride;4,7-EPOXYISOBENZOFURAN-1,3-DIONE,HEXAHYDRO-3A,7A-DIMETHYL-, (3A,4,7,7A)-;(3A-ALPHA,4B,7B,7A-ALPHA)-HEXAHYDRO-3A,7A-DIMETHYL-4,7-EPOXYISOBENZOFURAN-1,3-DIONE;(3AA,4B,7B,7AA)-HEXAHYDRO-3A,7A-DIMETHYL-4,7-EPOXYISOBENZOFURAN-1,3-DIONE;CANTHARIDIN;dimethyl-3,6-epoxyperhydrophthalic anhydride;HEXAHYDRO-3A,7A-DIMETHYL-4,7-EPOXYISOBENZO-FURAN-1,3-DIONE;;7-beta,7a-alpha)

CAS:56-25-7

MF:C10H12O4

MW:196.2

EINECS:200-263-3

Product Categories:chiral Cantharidin

Chemical Properties: mp 215-217 C(lit.) storage temp. Store at RT Merck 13,1757

CAS DataBase Reference: 56-25-7(

CAS DataBase Reference:) NIST Chemistry ReferenceCantharidin(56-25-7) EPA Substance Registry System4,7-Epoxyisobenzofuran- 1,3-dione, hexahydro-3a,7a-dimethyl-, (3aR,4S,7R,7aS)-rel-(56-25-7) T+,T Risk Statements 28-36/37/38-38-37-36-23/24/25 Safety Statements 53-45-36/37/39 RIDADR UN 2811 6.1/PG 1 WGK Germany 3 RTECS RN8575000 HazardClass 6.1(a) PackingGroup I Hazardous Substances Data56-25-7(Hazardous Substances Data) Dimethyl-3,6-epoxyperhydrophthalic anhydride Cantharidin

Usage And Synthesis:

Chemical Properties: white to light yellow crystal powde General DescriptionBrown to black

powder or plates or scales. Formerly used as a counterirritant and vesicant. Used for the removal of warts. Used as an experimental anti tumor agent. Active ingredient in spanish fly, a reputed aphrodisiac. Reactivity Profile Organic anhydrides, such as Cantharidin, are incompatible with acids, strong oxidizing agents, alcohols, amines, and bases. Health Hazard Cantharidin is classified as super toxic. Probable oral lethal dose in humans is less than 5 mg/kg or a taste of less than 7 drops for a 70 kg (150 lb.) person. It is very toxic by absorption through skin. Fire Hazard When heated to decomposition Cantharidin emits acrid smoke and irritating fumes. Biological Activity Natural toxin inhibitor of protein phosphatases 1 and 2A (K_i values are 1.1 and 0.19 μ M respectively); similar to okadaic acid (9,10-Deepithio-9,10-didehydroacanthifolicin). Displays > 500-fold selectivity over PP2B. Cantharidin

