



Formula: C₄₁H₆₄O₁₃

MW: 764.95

CAS: 71-63-6

TNP NUMBER: TNP00561

MDL NUMBER: MFCD08741664

IUPAC: 4-((1S,2S,5S,11S,7R,10R,14R,15R)-5-{5-[5-((2S,4S,5S,6R)-4,5-dihydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-yloxy))](4S,5S,2R,6R)-4-hydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-yloxy)](4S,5S,2R,6R)-4-hydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-yloxy)

Smiles:

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C1[C@H](O[C@@H]2O[C@@H]([C@H]([C@H](C2)O)O[C@@H]2O[C@@H]([C@H]([C@H](C2)O)O[C@@H]2O[C@@H]([C@H]([C@H](C2)O)O)C)C)C[C@H]2(CC[C@@H]3([C@@H]([C]2(C)C1)CC[C]1([C]3(CC[C@@H]1C1=CC(OC1)=O)O)C))
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Digitoxin 99%, Secondary glycoside from *Digitalis purpurea*, Scrophulariaceae

THERAPEUTIC CATEGORY: cardiotonic

ACCEPTORS: 13

DONORS: 5

ROTATION BONDS: 0

N+O: 13

Chiral Centers: 20

LogP: 4.64

LogS: -6.66

LIPINSKI: 2

Synonyms:

(3beta,5beta)-3-((o-2,6-dideoxy-beta-d-ribohexopyranosyl-(1-4)-o-2,6-dideoxy-be;(3beta,5beta)-hexopyranosyl)oxy]-14-hydroxy;(3beta,5beta)-y)-14-hydroxy;.4)-2,6-dideoxy-beta-D-ribo-hexopyranosyl)oxy]-14-hydroxy-, (3beta,5beta)-;.4)-O-2,6-dideoxy-beta-D-ribo-hexopyranosyl-(1.->3-((2,6-Dideoxy-4-O-[2,6-dideoxy-4-O-(2,6-dideoxyhexopyranosyl)hexopyranosyl]hexopyranosyl)oxy)-14-hydroxycard-20(22)-enolide;3-[(o-2,6-dideoxy-beta-d-ribo-hexopyranosyl-(1.fwdarw.4)-card-20(22)-enolid;4)-2,6-dideoxy-beta-D-ribo-hexopyranosyl)oxy]-14-hydroxy-, (3beta,5beta)-

CAS:71-63-6

MF:C41H64O13

MW:764.94

EINECS:200-760-5

Product Categories:Biochemistry;Glycosides;Steroidglycosides;Steroids;Sugars;Intermediates & Fine Chemicals;Pharmaceuticals;ATPase DIGITOXIN

Chemical Properties: mp 240 C (dec.)(lit.) refractive index 17 (C=2, CHCl3) storage temp. Dark Room solubility chloroform: soluble form powder Merck 3163 T Risk Statements 23/25-33 Safety Statements 45 RIDADR UN 2811 6.1/PG 1 WGK Germany 3 RTECS IH2275000 F 3-10 HazardClass 6.1(a) PackingGroup II DIGITOXIN

Usage And Synthesis:

Chemical Properties: White Solid UsageCardiotonic General DescriptionOdorless white or pale buff microcrystalline powder. Used as a cardiotonic drug. Health HazardMaterial is bioactive and capable of causing cardiac arrhythmias and electrolyte imbalances that may be fatal. Death is due to ventricular fibrillation or cardiac standstill. Material has a high toxicity hazard rating; it may cause death or permanent injury after a very short exposure. It is classified as super toxic; an estimated single lethal dose is 3-10 mg. Fire HazardWhen heated to decomposition, DIGITOXIN emits acrid smoke and irritating fumes. DIGITOXIN

