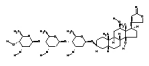

Formula: C41H64O14

MW: 780.95

CAS: 20830-75-6

TNP NUMBER: TNP00405

MDL NUMBER: MFCD03548112

IUPAC: 4-((1S,2S,5S,11S,15S,7R,10R,14R,16R)-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-yl

Smiles:
O1[C@H](C)[C@H]([C@@H](O)C[C@@H]1O[C@H]1(CC[C@@]2(C)[C@@H](CC[C@@H]3([C@@H]2(C[C@H]([C]2([C@]3(O)CC[C@@H]2(C2=CC(=O)OC2))C)O)))C1))O[C@@H]1O[C@@H]([C@H]([C@H](C1)O)O[C@@H]1O[C@@H]([C@H]([C@H](C1)O)O)C)C

Digoxin 95%

THERAPEUTIC CATEGORY: Cardiotonic

ACCEPTORS: 14

DONORS: 6

ROTATION BONDS: 0

N+O: 14

Chiral Centers: 21

LogP: 3.24

LogS: -6.23

LIPINSKI: 1

Synonyms:
(3beta,5beta,12beta)-3-((o-2,6-dideoxy-beta-d-ribo-hexapyranosyl-(1-4)-2,6-dide;-12,14-dihydroxycard-20(22)-enolide;14-dihydroxy-,(3beta,5beta,12beta)-xopyranosyl)oxy]-1;14-dihydroxy-,(3beta,5beta,12beta)-y)-1;-2,6-dideoxy-beta-d-ribo-hexopyranosyl-(1.fwdarw.)-2,6-dideoxy-beta-d-ribo-he;acygoxin;card-20(22)-enolide,3-((o-2,6-dideoxy-beta-d-ribo-hexopyranosyl-(1-4)-o-2,6-di;card-20(22)-enolide,3-[(o-2,6-dideoxy-beta-d-ribo-hexopyranosyl-(1.fwdarw.)-o

CAS:20830-75-5

MF:C41H64O14

MW:780.94

EINECS:244-068-1

Product Categories:Organics;Biochemistry;Glycosides;Steroidglycosides;Steroids;Sugars;Trisaccharides;Intermediates & Fine Chemicals;Pharmaceuticals;ATPase DIGOXIN

Chemical Properties: mp 248 C refractive index 12 (C=10, Pyridine) Merck 14,3167 EPA Substance Registry SystemCard-20(22)-enolide, 3-[(O-2,6-dideoxy-.beta.-D-ribo-hexopyranosyl-(1.fwdarw. 4)-O-2,6-dideoxy-.beta.-D- ribo-hexopyranosyl-(1.fwdarw. 4)-2,6-dideoxy-.beta.-D-ribo- hexopyranosyl)oxy]-12,14- dihydroxy-, (3.beta.,5.beta.,12.beta.)-(20830-75-5) T,T+ Risk Statements 25-26/27/28 Safety Statements 22-36/37/39-45 RIDADR UN 3462 6.1/PG 2 WGK Germany 3 RTECS IH6125000 F 3-10 HazardClass 6.1 PackingGroup II Hazardous Substances Data20830-75-5(Hazardous Substances Data) DIGOXIN

Usage And Synthesis:

Chemical Properties: White Crystalline Powder UsageCardiotonic General DescriptionClear to white crystals or white crystalline powder. Odorless. Used as a cardiotonic drug. Health HazardMaterial is a digitalis glycoside. Ingestion can cause death. Material is considered super toxic; probable human oral lethal dose is less than 5 mg/kg, a taste (less than 7 drops) for a 70 kg (150 lb.) person. Persons at risk include those taking drugs for thyroid and renal diseases.

Quinidine and diuretics taken concurrently with DIGOXIN can be hazardous. It should be used with extreme care during pregnancy and in nursing mothers. Fire HazardAvoid light. DIGOXIN