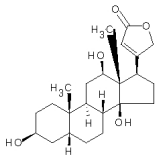

Formula: C23H34O5

MW: 390.52

CAS: 1672-46-4

MDL: MFCD03225464

TNP: TNP00235

DIGOXIGEN; DIGOXIGENIN; LANADIGENIN; LANADIGIGENIN;
20(22),5BETA-CARDENOLID-3BETA,12BETA,14BETA-TRIOL;
5BETA,20[22]-CARDENOLIDE-3BETA,12BETA,14-TRIOL;
5BETA,20[22]-CARDENOLIDE-3BETA,12BETA,14-TRIOL
3BETA,12BETA,14-TRIHYDROXY-5BETA,20[22]-CARDENOLIDE; 3BETA,12BET

LogP: 5.31

LogS: -5.67

Acceptors: 5

Donors: 3

Rotation Bonds: 0

Chiral Centers: 9

N+O: 5

LIPINSKY: 4

IUPAC: 4-((1S,2S,5S,11S,15S,7R,10R,14R,16R)-5,11,16-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0.0]heptadec-14-yl)-5-hydrofuran-2-one

Smiles:

C1([C@@H]2[C]3([C]([C@H]4([C@@H]([C]5(CC[C@@H](C[C@H]5(CC4))O)C)(C[C@H]3O)))(CC2)O)C)=CC(=O)OC1

Specification: DIGOXIGENIN Chemical Properties:

mp 222 C(lit.) Merck 13,3188 CAS DataBase Reference1672-46-4(CAS DataBase Reference) Safety Information Hazard Codes T+ Risk Statements 26/27/28 Safety Statements 36/37/39-45 RIDADR UN 2811 6.1/PG 1 WGK Germany 3 RTECS FH5390000 HazardClass 6.1(a) PackingGroup II DIGOXIGENIN Usage And Synthesis DIGOXIGENIN

Merck 13 Reference: Monograph Number: 0003188

Title: Digoxigenin

CAS Registry Number: 1672-46-4

CAS Name: (3b,5b,12b)-3,12,14-Trihydroxycard-20(22)-enolide

Additional Names: D20:22-3b,12b,14,21-tetrahydroxynorcholenic acid lactone; lanadigenin

Molecular Formula: C23H34O5

Molecular Weight: 390.51.

Percent Composition: C 70.74%, H 8.78%, O 20.49%

Literature References: The aglycone of digoxin. By hydrolysis of digoxin: Smith, J. Chem. Soc. 1930, 508. From Digitalis orientalis L. and D. lanata Ehrh., Scrophulariaceae: Mannick, Schneider, Arch. Pharm. 279, 223 (1941); Pataki et al., Helv. Chim. Acta 36, 1295 (1953). Structure: Meyer, Reichstein, Experientia 9, 253 (1953); Cardwell, Smith, ibid. 367; eidem, J. Chem. Soc. 1954, 2012. Synthesis: P. Welzel, H. Stein, Tetrahedron Lett. 22, 3385 (1981).

Derivative Type: Dihydrate

Properties: Prismatic rods from dil alc. Anhydr as stout prisms from ethyl acetate, mp 222. [a]20546 +27.0 (c = 1.77 in methanol). Although it is a 3b-alcohol, it is not precipitated by digitonin (Pataki).

Melting point: mp 222

Optical Rotation: [a]20546 +27.0 (c = 1.77 in methanol)

Derivative Type: 3,12-Diacetyldigoxigenin

Properties: Prisms from dil methanol, mp 222-223. [a]20546 +61.3 (c = 2 in methanol).

Melting point: mp 222-223

Optical Rotation: [a]20546 +61.3 (c = 2 in methanol)