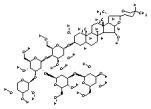

Formula: C56H92O29

MW: 1229.33

CAS: 11024-24-1

MDL: MFCD08741672

TNP: TNP00392

(2.alpha.,3.beta.,5.alpha.,15.beta.,25R)-2,15-dihydroxyspirostan-3-ylO-.beta.-D-glucopyranosyl-(1.beta.-D-Galactopyranoside;
beta-d-galactopyranoside,(2alpha,3beta,5alpha,15beta,25theta)-2,15-dihyd;
osyl-(1.fwdarw.2)-o-[beta-d-xylopyranosyl-(1.fwdarw.3)]-o-

LogP: 2.65

LogS: -4.38

Acceptors: 29

Donors: 17

Rotation Bonds: 4

Chiral Centers: 38

N+O: 29

LIPINSKY: 1

Info: Digitonin, clinical reagent. Chlestrerol determination

IUPAC: 6-(6-{2-[(2R,3R,4R,5R,6R)-6-((8S,9S,13S,15S,18S,19S,24S,7R,10R,12R,14R,21R,22R)-9,21-dihydroxy-3,13,15,19-tetramethyl-11-oxaspiro[2H-3,4,5,6-tetrahydropyran-6,6'-pentacyclo[10.8.0.0.0.0]icosane]-22-yloxy)-4,5-dihydrox

y-2-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-3-yl)oxy]-4-((2S,4S,3R,5R)-3,4,
5-trihydroxy(2H-3,4,5,6-tetrahydropyran-2-yl)oxy)(2S,4S,5S,3R,6R)-5-hydroxy-6-
(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-3-yloxy)}(3S,4S,6S,2R,5R)-3,5-dihyd
roxy-2-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-4-yloxy))(3S,4S,6S,2R,5R)-2-
(hydroxymethyl)-2H-3,4,5,6-tetrahydropyran-3,4,5-triol

Smiles:
C1[C@@H](O[C@H]2[C@@H]([C@H]([C@H]([C@H](O2)CO)O[C@H]2[C@@H]([C@H]([C@
@H]([C@H](O2)CO)O)O[C@H]2[C@@H]([C@H]([C@@H](CO2)O)O)O)O[C@H]2[C@@H]([C
@H]([C@@H]([C@H](O2)CO)O)O[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O)O)
O)O)[C@H](O)C[C]2(C)[C@H]1CC[C@@H]1[C@@H]2CC[C@@]2([C@H]3([C@H](C)[C@]4(
OCC(CC4)C)O[C@H]3([C@H]([C@@H]12)O)))C

Specification: Nonionic Surfactants (for Biochemistry); Biochemistry; Glycosides; Steroidglycosides; Steroids; Sugars; Surfactants (for Biochemistry) DIGITONIN Chemical Properties:

 mp 230-240 C (dec.)(lit.) refractive index -52 (C=1, EtOH) storage temp. Store at RT. solubility H2O: 10 mg/mL at 95 C hot, clear, colorless color white Merck 3161 Safety Information Hazard Codes T Risk Statements 23/24/25 Safety Statements 22-28-36/37-45 RIDADR UN 3462 6.1/PG 3 WGK Germany 3 RTECS IH2050050 F 3-10 HazardClass 6.1(a) PackingGroup IIDIGITONIN Usage And Synthesis Chemical Properties:

white crystalline powder General DescriptionCrystals or white powder. Air & Water ReactionsForms soapy aqueous suspension . Reactivity ProfileDIGITONIN is incompatible with strong oxidizing agents and strong acids. (NTP, 1992 Fire HazardFlash point data for DIGITONIN are not available; however, DIGITONIN is probably combustible. DIGITONIN

Merck 13 Reference: Monograph Number: 0003183

Title: Digitonin

CAS Registry Number: 11024-24-1

Additional Names: Digitin

Molecular Formula: C56H92O29

Molecular Weight: 1229.31.

Percent Composition: C 54.71%, H 7.54%, O 37.74%

Literature References: Obtained from the seeds of Digitalis purpurea L., Scrophulariaceae. Extraction procedure: Gisvold, J. Am. Pharm. Assoc. 23, 664 (1934). Purification of commercial digitonin and its separation into two fractions: G. Ruhenstroth-Bauer, P. M. Breitenfeld, Z. Physiol. Chem. 302, 111 (1955). Structure: Tschesche, Wulff, Tetrahedron 19,

621 (1963). Use as clinical reagent: H. H. Leffler, Am. J. Clin. Pathol. 31, 310 (1959).

Properties: Crystals from alc, sinters 225. Indistinct mp 235-240. [a]D20 -54 (0.45 g in 15.8 ml methanol). One gram dissolves in 57 ml abs alc, in 220 ml 95% alc. Practically insol in water, forming a soapy suspension. Also practically insol in chloroform, ether.

Melting point: Indistinct mp 235-240

Optical Rotation: [a]D20 -54 (0.45 g in 15.8 ml methanol)

Use: Clinical reagent (cholesterol determination).