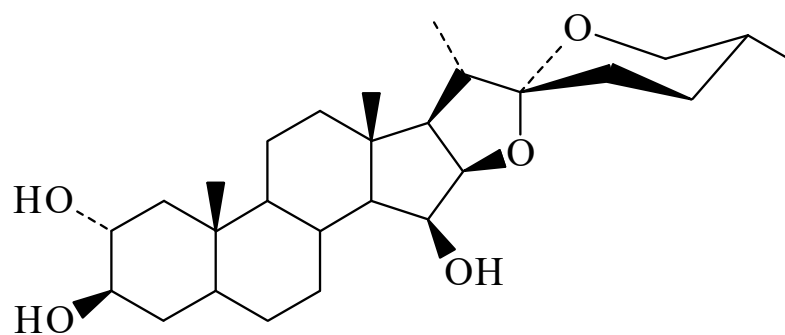




>>Entry Name: Spirostane-2,3,15-triol



Molecular Formula: C₂₇H₄₄O₅

Molecular Weight: 448.642

Accurate Mass: 448.318875

Percentage Composition: C 72.28%; H 9.88%; O 17.83%

>>Variant: (2 α ,3 β ,5 α ,15 β ,25*R*)-form

Synonym(s): Digitogenin

CAS Registry Number: 511-34-2

Molecular Formula: C₂₇H₄₄O₅

Molecular Weight: 448.642

Accurate Mass: 448.318875

Percentage Composition: C 72.28%; H 9.88%; O 17.83%

Biological Source: Aglycone from *Digitalis purpurea*, also occurring in free state. Also in *Digitalis lanata*, *Digitalis ciliata* and *Cestrum parqui*

Physical Description: Needles (MeOH)

Melting Point: Mp 296° (280-283°)

Optical Rotation: [α]_D¹⁹ -81 (CHCl₃)

>>Derivative: 3-*O*-[β -D-Glucopyranosyl-(1 $\rightarrow$ 3)- β -D-galactopyranosyl-(1 $\rightarrow$ 2)-[β -D-xylopyranosyl-(1 $\rightarrow$ 3)]-*O*- β -D-glucopyranosyl-(1 $\rightarrow$ 4)- β -D-galactopyranoside]

Synonym(s): Digitonin

CAS Registry Number: 11024-24-1

Molecular Formula: C₅₆H₉₂O₂₉

Molecular Weight: 1229.325

Accurate Mass: 1228.572435

Percentage Composition: C 54.71%; H 7.54%; O 37.74%

Biological Source: Constit. of *Digitalis purpurea* and other *Digitalis* spp.

Use/Importance: Used as an aq. soln. for detn. of cholesterol

Physical Description: Cryst. (EtOH)

Melting Point: Mp 235-240°

Optical Rotation: [α]_D -54.3 (MeOH)

Other Data: Forms 1:1 insol. complex with cholesterol

Aldrich: 26074-6

Fluka: 37010

Sigma: D5628

>>Derivative: 3-*O*-[β -D-Galactopyranosyl-(1 $\rightarrow$ 2)-[β -D-xylopyranosyl-(1 $\rightarrow$ 3)]-*O*- β -D-glucopyranosyl-(1 $\rightarrow$ 4)- β -D-galactopyranoside]

Synonym(s): Desglucodigitonin

Molecular Formula: C₅₀H₈₂O₂₄

Molecular Weight: 1067.183

Accurate Mass: 1066.51961

Percentage Composition: C 56.27%; H 7.74%; O 35.98%

Physical Description: Fine needles + 2H₂O (1-butanol aq.)

Melting Point: Mp 243-245°

Optical Rotation: [α]_D²⁰ -71.4 (c, 0.28 in Py)