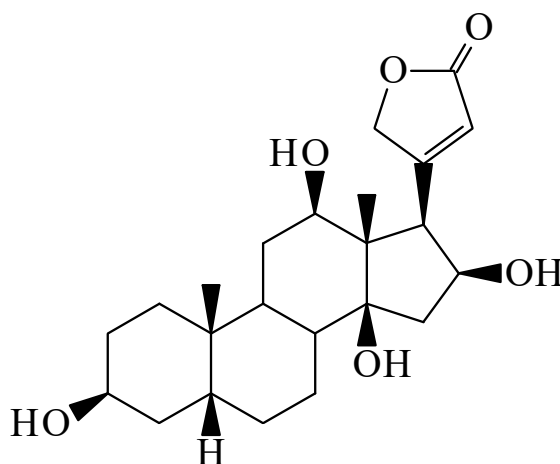




>>Entry Name: 3,12,14,16-Tetrahydroxycard-20(22)-enolide



Molecular Formula: C₂₃H₃₄O₆

Molecular Weight: 406.518

Accurate Mass: 406.23554

Percentage Composition: C 67.96%; H 8.43%; O 23.61%

>>Variant: (3β,5β,12β,14β,16β)-form

Synonym(s): Diginatigenin

CAS Registry Number: 559-57-9

Molecular Formula: C₂₃H₃₄O₆

Molecular Weight: 406.518

Accurate Mass: 406.23554

Percentage Composition: C 67.96%; H 8.43%; O 23.61%

Biological Source: Constit. of *Digitalis lanata*

Physical Description: Cryst. (H₂O)

Melting Point: Mp 157° (115-130 and 196-200°)

Optical Rotation: [α]_D²⁰ +34 (MeOH)

>>Derivative: 3-*O*-Digitoxoside

Synonym(s): Diginatin

CAS Registry Number: 52589-12-5

Molecular Formula: C₂₉H₄₄O₉

Molecular Weight: 536.661

Accurate Mass: 536.298535

Percentage Composition: C 64.90%; H 8.26%; O 26.83%

Biological Source: Constit. of *Digitalis lanata*

Use/Importance: Cardiac glycoside

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 234°

Optical Rotation: [α]_D²⁷ +23.7 (c, 2.2 in MeOH)

Calculated Log P Data: Log P -2.39 (uncertain value) (calc)

>>Derivative: 3-*O*-[3-*O*-Acetyl-D-digitoxosido(1→4)-D-digitoxosyl(1→4)-D-digitoxoside]

Synonym(s): Acetyldiginatin α

Molecular Formula: C₄₃H₆₆O₁₆

Molecular Weight: 838.985

Accurate Mass: 838.43509

Percentage Composition: C 61.56%; H 7.93%; O 30.51%

Biological Source: Identified in leaves of *Digitalis lanata* (poss. as mixt. with other isomers of acetyldiginatin)

Physical Description: Platelets (MeOH/CHCl₃/Et₂O)

Melting Point: Mp 199-202°

Optical Rotation: [α]_D²⁰ +30.1 (c, 0.6 in Py)