



>>>Derivative: 3-*O*-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→4)-2,6-dideoxy-3-*O*-methyl-β-D-*ribo*-hexopyranoside]

Synonym(s): 17α-Digitoxigenin gentiobiosylcymaroside

CAS Registry Number: 129830-68-8

Molecular Formula: C₄₂H₆₆O₁₇

Molecular Weight: 842.973

Accurate Mass: 842.430005

Percentage Composition: C 59.84%; H 7.89%; O 32.27%

Biological Source: Isol. from *Beaumontia brevitiba*

Physical Description: Solid

Optical Rotation: [α]_D²⁶+2 (c, 0.4 in MeOH)

>>>Derivative: 3-Ac

Molecular Formula: C₂₅H₃₆O₅

Molecular Weight: 416.556

Accurate Mass: 416.256275

Percentage Composition: C 72.09%; H 8.71%; O 19.20%

Melting Point: Mp 170°. Mp 242-244° (double Mp)

Optical Rotation: [α]_D²¹+27.4 (CHCl₃)

>>>Variant: (3β,5β,14β,17β)-form

Synonym(s): Digitoxigenin. Thevetigenin. Cerberigenin. Echujetin

CAS Registry Number: 143-62-4

Molecular Formula: C₂₃H₃₄O₄

Molecular Weight: 374.519

Accurate Mass: 374.24571

Percentage Composition: C 73.76%; H 9.15%; O 17.09%

Biological Source: Widely distributed aglycone. Found in the Scrophulariaceae, Asclepiadaceae, Apocynaceae and Periplocaceae

Biological Use/Importance: Cardiotonic agent

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 253°

Optical Rotation: [α]_D¹⁷+19.1 (c, 1.4 in MeOH)

Hazard & Toxicity: LD₅₀ (mus, orl) 26.2 mg/kg

>>>Derivative: 3-*O*-β-D-Allopyranoside

CAS Registry Number: 148092-06-2

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 the defence secretion of the beetle *Oreina gloriosa*

>>>Derivative: 3-*O*-(2,3-Dideoxy-α-L-rhamnopyranoside)

Synonym(s): Ramnodigin, INN

CAS Registry Number: 33156-28-4

Molecular Formula: C₂₉H₄₄O₆

Molecular Weight: 488.663

Accurate Mass: 488.31379

Percentage Composition: C 71.28%; H 9.08%; O 19.64%

Biological Use/Importance: Cardiotonic agent

Development Status: Never marketed

Melting Point: Mp 218°

Optical Rotation: [α]_D²⁰-41 (c, 0.5 in MeOH)

Calculated Log P Data: Log P 3.01 (uncertain value) (calc)