



Accurate Mass: 712.36701

Percentage Composition: C 60.66%; H 7.92%; O 31.42%

Biological Source: Constit. of *Digitalis purpurea*, many other *Digitalis* spp., *Nerium* spp., *Adenium bohemianum*, *Cryptostegia grandiflora* and others

Physical Description: Cryst.

Melting Point: Mp 243.3-244 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -1.1$ (c, 0.9 in MeOH)

Sigma: D0891

>> **Derivative:** 3-*O*-[β-D-Glucopyranosyl-(1→2)-6-deoxy-3-*O*-methyl-β-D-glucopyranoside]

Synonym(s): Neodigitalinum verum

Molecular Formula: C₃₆H₅₆O₁₄

Molecular Weight: 712.83

Accurate Mass: 712.36701

Percentage Composition: C 60.66%; H 7.92%; O 31.42%

Biological Source: Isol. from leaves of *Digitalis lanata*, also from *Digitalis parviflora* and *Digitalis grandiflora*

Physical Description: Cryst. + 2H₂O (EtOH/Et₂O)

Melting Point: Mp 220-225°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +3$ (EtOH)

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

Synonym(s): Glucogitoroside

CAS Registry Number: 663-16-1

Molecular Formula: C₃₅H₅₄O₁₃

Molecular Weight: 682.804

Accurate Mass: 682.356445

Percentage Composition: C 61.57%; H 7.97%; O 30.46%

Biological Source: Constit. of *Digitalis lanata*

Physical Description: Powder (MeOH/dimethyl carbonate)

Melting Point: Mp 212-216°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +19.9$ (c, 0.7 in EtOH)

>> **Derivative:** 3-*O*-[β-D-Glucopyranosyl-(1→4)-2,3-di-*O*-methyl-β-D-glucopyranoside]

Synonym(s): Glucogitodimethoside

Molecular Formula: C₃₇H₅₈O₁₅

Molecular Weight: 742.856

Accurate Mass: 742.377575

Percentage Composition: C 59.82%; H 7.87%; O 32.31%

Biological Source: Isol. from root bark of *Streblus asper*

Physical Description: Glass

Optical Rotation: $[\alpha]_{\text{D}}^{23} -21.5$ (c, 0.21 in MeOH)

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

Synonym(s): Gitoxin. Anhydrogitalin. Bigitalin. Gitoxoside

CAS Registry Number: 4562-36-1

Molecular Formula: C₄₁H₆₄O₁₄

Molecular Weight: 780.948

Accurate Mass: 780.42961

Percentage Composition: C 63.06%; H 8.26%; O 28.68%

Biological Source: Constit. of *Digitalis* spp.

Physical Description: Cryst.

Melting Point: Mp 282-285 dec.° (266-269°)

Optical Rotation: $[\alpha]_{\text{D}}^{24} +5$ (c, 1 in Py). $[\alpha]_{\text{D}} +22$ (CHCl₃)

Hazard & Toxicity: LD₅₀ (gpg, ivn) 68 mg/kg

Rare Chemicals Library: S40421-7

Sigma: G5381