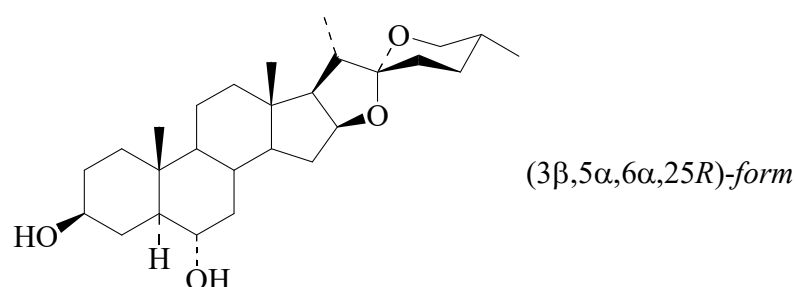




>>Entry Name: Spirostane-3,6-diol, 9Cl



Molecular Formula: C₂₇H₄₄O₄

Molecular Weight: 432.642

Accurate Mass: 432.32396

Percentage Composition: C 74.96%; H 10.25%; O 14.79%

>>Variant: (3β,5α,6α,25R)-form

Synonym(s): Chlorogenin

CAS Registry Number: 562-34-5

Molecular Formula: C₂₇H₄₄O₄

Molecular Weight: 432.642

Accurate Mass: 432.32396

Percentage Composition: C 74.96%; H 10.25%; O 14.79%

Biological Source: Sapogenin from *Chlorogalum pomeridianum*. Also in *Agave* and *Yucca* spp. and *Furcraea gigantea*

Biological Use/Importance: Antiinflammatory agent

Physical Description: Cryst. (MeOH aq.), needles (CHCl₃)

Melting Point: Mp 275-276°

Optical Rotation: [α]_D²⁵ -64 (CHCl₃)

Calculated Log P Data: Log P 4.21 (uncertain value) (calc)

>>Derivative: 3-O-[β-D-Xylopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]

CAS Registry Number: 310883-01-3

Molecular Formula: C₅₅H₉₀O₂₇

Molecular Weight: 1183.3

Accurate Mass: 1182.566955

Percentage Composition: C 55.83%; H 7.67%; O 36.51%

Biological Source: Constit. of *Polianthes tuberosa*

Physical Description: Amorph. solid

Optical Rotation: [α]_D²⁷ -42 (c, 0.1 in MeOH)

>>Derivative: Di-Ac

CAS Registry Number: 3514-58-7

Molecular Formula: C₃₁H₄₈O₆

Molecular Weight: 516.717

Accurate Mass: 516.34509

Percentage Composition: C 72.06%; H 9.36%; O 18.58%

Melting Point: Mp 153-155°

Optical Rotation: [α]_D²⁰ -38 (c, 1.0 in CHCl₃)

>>Derivative: 3,6-Diketone

Synonym(s): Spirostane-3,6-dione. **Chlorogenone**

CAS Registry Number: 3514-59-8

Molecular Formula: C₂₇H₄₀O₄

Molecular Weight: 428.611

Accurate Mass: 428.29266

Percentage Composition: C 75.66%; H 9.41%; O 14.93%

Biological Source: Isol. from fruits of *Solanum torvum*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 243.5-244.5° (233-236°)