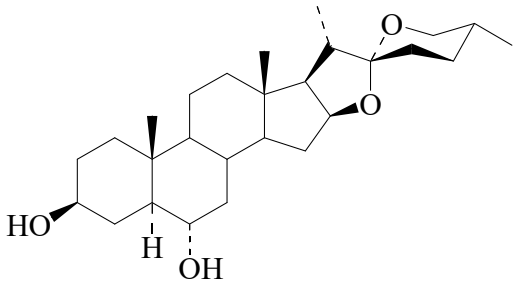
>>**Entry Name: Spirostane-3,6-diol,** 9CI



(3β,5α,6α,25*R*)-*form*

Molecular Formula: $C_{27}H_{44}O_4$
Molecular Weight: 432.642
Accurate Mass: 432.32396
Percentage Composition: C 74.96%; H 10.25%; O 14.79%

>>**Variant:** (3β,5α,6α,25*R*)-form
Synonym(s): Chlorogenin

CAS Registry Number: 562-34-5

Molecular Formula: $C_{27}H_{44}O_4$
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 ($CHCl_3$)
Melting Point: Mp 275-276°
Optical Rotation: $[\alpha]_D^{25}$ –64 ($CHCl_3$)
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: $C_{55}H_{90}O_{27}$
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: $[\alpha]_D^{27}$ –42 (c, 0.1 in MeOH)

>>**Derivative:** Di-Ac

CAS Registry Number: 3514-58-7
Molecular Formula: $C_{31}H_{48}O_6$
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: $[\alpha]_D^{20}$ –38 (c, 1.0 in $CHCl_3$)

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

CAS Registry Number: 3514-59-8
Molecular Formula: $C_{27}H_{40}O_4$
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. (Me_2CO)
Melting Point: Mp 243.5-244.5° (233-236°)