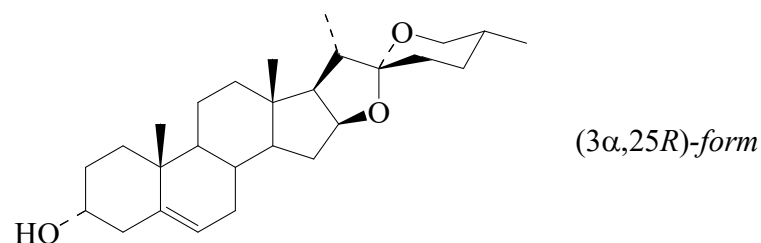




>>Entry Name: Spirost-5-en-3-ol



Related CAS Registry Numbers(s): 53846-52-9

Molecular Formula: C₂₇H₄₂O₃

Molecular Weight: 414.627

Accurate Mass: 414.313395

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

>>Variant: (3 α ,25*R*)-form

Synonym(s): 3-Epidiosgenin

CAS Registry Number: 66289-52-9

Molecular Formula: C₂₇H₄₂O₃

Molecular Weight: 414.627

Accurate Mass: 414.313395

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

Biological Source: Isol. from the crude drug Sensokushichikon

Physical Description: Cryst.

Melting Point: Mp 244-246°

Optical Rotation: [α]_D -145

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

CAS Registry Number: 66289-51-8

Molecular Formula: C₃₃H₅₂O₈

Molecular Weight: 576.769

Accurate Mass: 576.36622

Percentage Composition: C 68.72%; H 9.09%; O 22.19%

Biological Source: Constit. of *Gynura japonica*

Physical Description: Cryst.

Melting Point: Mp 218-221°

Optical Rotation: [α]_D -122

>>Variant: (3 β ,25*R*)-form

Synonym(s): Diosgenin. Nitogenin. Dioscorea sapogenin

CAS Registry Number: 512-04-9

Molecular Formula: C₂₇H₄₂O₃

Molecular Weight: 414.627

Accurate Mass: 414.313395

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

Biological Source: Sapogenin from *Dioscorea* spp., *Solanum* spp. *Trillium erectum*, *Balanites aegyptica*, *Aletris farinosa*, *Clintonia* spp. and many other plants

Use/Importance: Starting material for preparation of pregnane derivatives

Biological Use/Importance: Antiinflammatory, estrogenic agent

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 204-207°

Optical Rotation: [α]_D²⁵ -129 (c, 1.4 in CHCl₃)

Solubility: Sol. MeOH, CHCl₃; poorly sol. H₂O

Calculated Log P Data: Log P 5.82 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (rat, ipr) 4872 mg/kg. LD₅₀ (mus, orl) >8000 mg/kg. LD₅₀ (mus, ipr) 4000 mg/kg

Fluka: 42499

Rare Chemicals Library: S37385-0

Sigma: D1634