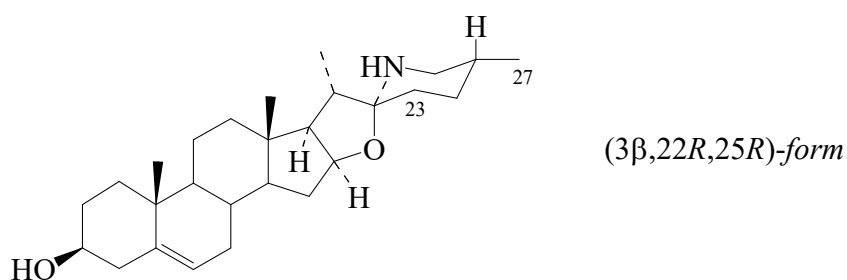




>>Entry Name: Spirosol-5-en-3-ol



Molecular Formula: C₂₇H₄₃NO₂

Molecular Weight: 413.642

Accurate Mass: 413.329379

Percentage Composition: C 78.40%; H 10.48%; N 3.39%; O 7.74%

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

Sigma: S0888

>>Variant: (3β,22R,25R)-form

Synonym(s): Solasodine. Solancarpidine. Purapuridine. Solanidine S. Solancarpine

CAS Registry Number: 126-17-0

Molecular Formula: C₂₇H₄₃NO₂

Molecular Weight: 413.642

Accurate Mass: 413.329379

Percentage Composition: C 78.40%; H 10.48%; N 3.39%; O 7.74%

Biological Source: Isol. from *Solanum aculeatissimum*, *Solanum cyananthum*, *Cestrum purpureum* and other plants, v. widely distributed in the Solanaceae as the alkamine constit. of glycoside alkaloids

Use/Importance: Much investigated as potential starting material for coml. steroid synth, as alternative to [HKK91-O](#)

Biological Use/Importance: Antineoplastic agent. Also reputed to have antiandrogenic, antiinflammatory and antispermatogenic props.

Melting Point: Mp 200-201°

Optical Rotation: [α]_D -98 (MeOH)

Calculated Log P Data: Log P 5.59 (uncertain value) (calc)

Other Data: Dimorph., both forms with same Mp

Hazard & Toxicity: LD₅₀ (rat, orl) 4978 mg/kg. Exp. reprod. and teratogenic effects

>>Derivative: Hydrochloride

Melting Point: Mp 313-314°

>>Derivative: Picrate

Melting Point: Mp 144-145°

>>Derivative: 3-O-β-D-Glucopyranoside

Synonym(s): Solasodine 3-O-β-D-glucopyranoside

CAS Registry Number: 14197-65-0

Molecular Formula: C₃₃H₅₃NO₇

Molecular Weight: 575.784

Accurate Mass: 575.382204

Percentage Composition: C 68.84%; H 9.28%; N 2.43%; O 19.45%

Biological Source: Alkaloid from whole plants of *Solanum umbelliferum*

Physical Description: Amorph. powder

Melting Point: Mp 246-248°

Optical Rotation: [α]_D²⁶ -81.1 (c, 0.24 in MeOH)