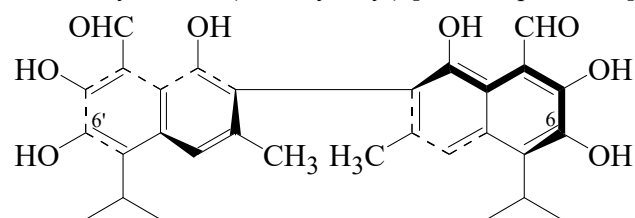




>>Entry Name: Gossypol

Synonym(s): 1,1',6,6',7,7'-Hexahydroxy-3,3'-dimethyl-5,5'-bis(1-methylethyl)-[2,2'-binaphthalene]-8,8'-dicarboxaldehyde, 9Cl. Thespesin



Absolute
Configuration

CAS Registry Number: 303-45-7

Related CAS Registry Numbers(s): 62770-38-1

Molecular Formula: C₃₀H₃₀O₈

Molecular Weight: 518.562

Accurate Mass: 518.19407

Percentage Composition: C 69.49%; H 5.83%; O 24.68%

Biological Use/Importance: Exhibits antifertility activity. Antispermato-genic props. Antineoplastic agent, potential treatment for gliomas. Shows anti-HIV activity

Development Status: Has undergone widespread trials in Peoples Republic of China. Toxicity and poor therapeutic potential has precluded further interest as a male contraceptive

Solubility: BERDY SOL: Poorly sol. H₂O

Calculated Log P Data: Log P 7.06 (uncertain value) (calc)

UV: [neutral] λ_{max} 237 (ε 60250); 277 (ε 26300); 375 (ε 15850) (MeOH) (Berdy)

Sigma: G8761

>>Variant: (+)-form

CAS Registry Number: 20300-26-9

Molecular Formula: C₃₀H₃₀O₈

Molecular Weight: 518.562

Accurate Mass: 518.19407

Percentage Composition: C 69.49%; H 5.83%; O 24.68%

Biological Source: Constit. of *Azanza* spp., *Cienfuegosia* sp., *Gossypium* spp., *Montezuma* sp. and *Thespesia* sp.

Physical Description: Pale yellow needles (petrol), deep-yellow prisms + Me₂CO (Me₂CO), large elongated plates (Me₂CO aq.)

Melting Point: Mp 181-183°

Optical Rotation: [α]_D¹⁹ +445 (c, 0.15 in CHCl₃)

Hazard & Toxicity: LD₅₀ (mus, ipr) 35 mg/kg. Exp. reprod. effects

>>Derivative: Hexa-Me ether

CAS Registry Number: 17273-30-2

Melting Point: Mp 242-244°

Optical Rotation: [α]_D +177 (CHCl₃)

>>Variant: (-)-form

CAS Registry Number: 90141-22-3

Molecular Formula: C₃₀H₃₀O₈

Molecular Weight: 518.562

Accurate Mass: 518.19407

Percentage Composition: C 69.49%; H 5.83%; O 24.68%

Biological Source: Constit. of *Gossypium arboreum*, *Gossypium barbadense* and *Gossypium hirsutum*

Physical Description: Cryst.

Melting Point: Mp 178-183°

Optical Rotation: [α]_D²⁶ -360 (86% ee)

Other Data: More pharmacol. active isomer