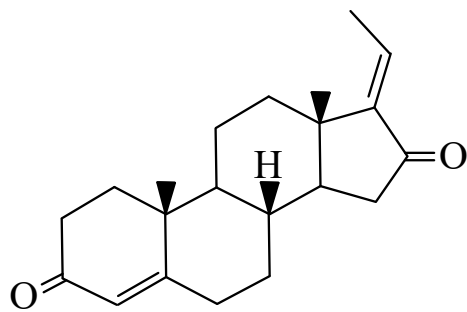




>>Entry Name: Pregna-4,17(20)-diene-3,16-dione, 9Cl

Synonym(s): Guggulsterone. Guggulipid



(*E*)-form

CAS Registry Number: 95975-55-6

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Use/Importance: Antihyperlipidaemic agent

Calculated Log P Data: Log P 3.53 (uncertain value) (calc)

>>Variant: (*E*)-form

CAS Registry Number: 39025-24-6

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Biological Source: Constit. of *Commiphora mukul* and *Ailanthus grandis*

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 168-170°

Optical Rotation: [α]_D -28.4 (c, 2.1 in CHCl₃)

>>Variant: (*Z*)-form

CAS Registry Number: 39025-23-5

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Biological Source: Constit. of *Commiphora mukul* and *Ailanthus grandis*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 192-193°

Optical Rotation: [α]_D -77.1 (c, 2.1 in CHCl₃)

References:

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Patil, V.D. *et al.*, *Tetrahedron*, 1972, **28**, 2341

Kakrani, H.K., *Indian Drugs*, 1981, **18**, 417, (*rev, props, uses*)

Satyavati, G.V., *Econ. Med. Plant Res.*, 1991, **5**, 47, (*rev*)

Singh, R.B. *et al.*, *Cardiovasc. Drug Ther.*, 1994, **8**, 659, (*use*)

Hung, T. *et al.*, *Phytochemistry*, 1995, **39**, 1403, (*isol, pmr, cmr, cryst struct*)