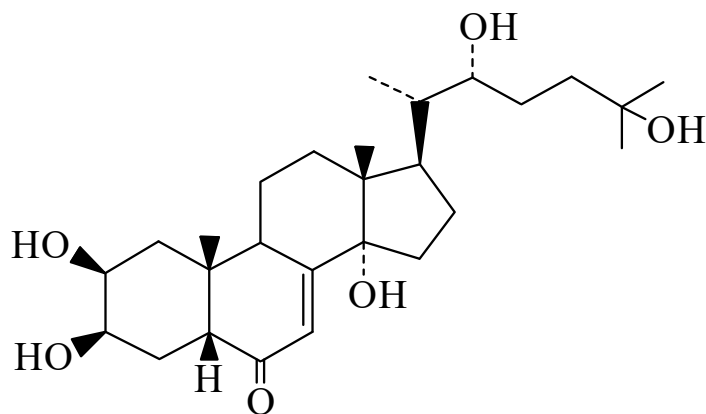




>>Entry Name: 2,3,14,22,25-Pentahydroxycholest-7-en-6-one



Molecular Formula: C₂₇H₄₄O₆

Molecular Weight: 464.641

Accurate Mass: 464.31379

Percentage Composition: C 69.80%; H 9.54%; O 20.66%

>>Variant: (2β,3β,5β,22R)-form

Synonym(s): α-Ecdysone. Ecdysone

CAS Registry Number: 3604-87-3

Molecular Formula: C₂₇H₄₄O₆

Molecular Weight: 464.641

Accurate Mass: 464.31379

Percentage Composition: C 69.80%; H 9.54%; O 20.66%

Biological Source: Moulting hormone of silkworm pupae. Isol. from various plants e.g. ferns

Physical Description: Cryst. (THF/petrol)

Melting Point: Mp 242°

Optical Rotation: [α]_D²⁶+64.7 (c, 1 in EtOH)

Aldrich: 36042-2

Sigma: E9004

>>Derivative: 22-Sulfate, Na salt

Synonym(s): α-Ecdysone 22-sulfate

Molecular Formula: C₂₇H₄₃NaO₉S

Molecular Weight: 566.687

Accurate Mass: 566.252547

Percentage Composition: C 57.23%; H 7.65%; Na 4.06%; O 25.41%; S 5.66%

Biological Source: Constit. of *Silene brahuica*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 224-226°

Optical Rotation: [α]_D²⁰+63.3 (c, 0.91 in MeOH)

References:

- Karlson, P. *et al.*, *Chem. Ber.*, 1965, **98**, 2394, (*struct*)
Huber, R. *et al.*, *Chem. Ber.*, 1965, **98**, 2403, (*cryst struct*)
Kerb, U. *et al.*, *Helv. Chim. Acta*, 1966, **49**, 1601, (*synth*)
Siddall, J.B. *et al.*, *J.A.C.S.*, 1966, **88**, 862, (*synth*)
Mori, H. *et al.*, *Chem. Pharm. Bull.*, 1968, **16**, 563, (*synth*)
Chang, Y.K. *et al.*, *Chem. Comm.*, 1970, 1217, (*isol, struct*)
Koreeda, M. *et al.*, *J.A.C.S.*, 1971, **93**, 4084, (*config*)
Nakanishi, K., *Pure Appl. Chem.*, 1971, **25**, 167, (*rev*)
Hikino, H. *et al.*, *Chem. Pharm. Bull.*, 1975, **23**, 125, (*cmr*)
Lee, E. *et al.*, *J.A.C.S.*, 1976, **98**, 1634, (*synth*)
Krepinsky, J. *et al.*, *Org. Magn. Reson.*, 1977, **10**, 25, (*cmr*)
Tsoupras, G. *et al.*, *Tetrahedron*, 1983, **39**, 1789, (*conjugates*)
Saatov, Z. *et al.*, *Khim. Prir. Soedin.*, 1984, **20**, 467; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 441, (*isol*)
Koolman, J., *Ecdysone*, Thieme, 1989, 74; *CA*, **112**, 217330y, (*rev*)
Coll, J. *et al.*, *Tetrahedron*, 1994, **50**, 7247, (*isol, cmr*)
Devarenne, T.P. *et al.*, *Phytochemistry*, 1995, **40**, 1125, (*biosynth*)
Blais, C. *et al.*, *Biochem. J.*, 1996, **320**, 413, (*biosynth*)