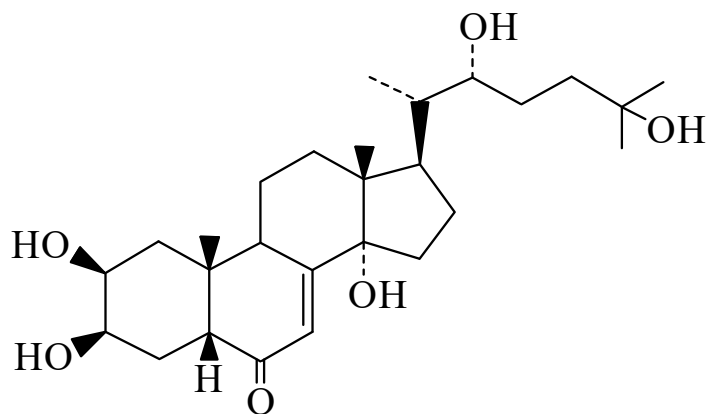




>>Entry Name: 2,3,14,22,25-Pentahydroxycholest-7-en-6-one



**Molecular Formula:** C<sub>27</sub>H<sub>44</sub>O<sub>6</sub>

**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:** C<sub>27</sub>H<sub>44</sub>O<sub>6</sub>

**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]<sub>D</sub><sup>26</sup>+64.7 (c, 1 in EtOH)

**Aldrich:** 36042-2

**Sigma:** E9004

>>Derivative: 22-Sulfate, Na salt

**Synonym(s):** α-Ecdysone 22-sulfate

**Molecular Formula:** C<sub>27</sub>H<sub>43</sub>NaO<sub>9</sub>S

**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]<sub>D</sub><sup>20</sup>+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*)