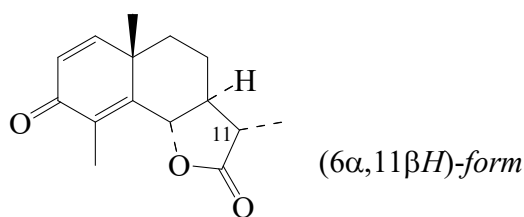




>>Entry Name: 3-Oxo-1,4-eudesmadien-12,6-olide



**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>3</sub>

**Molecular Weight:** 246.305

**Accurate Mass:** 246.125595

**Percentage Composition:** C 73.15%; H 7.37%; O 19.49%

**Biological Use/Importance:** Anthelmintic agent. Used in treatment of nervous complaints

**Calculated Log P Data:** Log P 1.38 (calc)

>>Variant: (6 $\alpha$ ,11 $\beta$ H)-form

**Synonym(s):**  $\alpha$ -Santonin. Santonin

**CAS Registry Number:** 481-06-1

**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>3</sub>

**Molecular Weight:** 246.305

**Accurate Mass:** 246.125595

**Percentage Composition:** C 73.15%; H 7.37%; O 19.49%

**Biological Source:** Occurs widely in plants, especially *Artemisia* spp.

**Physical Description:** Cryst. (H<sub>2</sub>O, EtOH or Et<sub>2</sub>O)

**Melting Point:** Mp 174-176°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>18</sup> -173 (EtOH)

**Calculated Log P Data:** Log P 1.38 (calc)

**Other Data:** Chemistry, esp. photochemistry, extensively investigated. Pharmacol. active isomer

**Hazard & Toxicity:** LD<sub>50</sub> (mus, orl) 900 mg/kg. Toxic human effects including visual disturbance

**Aldrich:** 22308-5

**Fluka:** 84508

**Rare Chemicals Library:** S57940-8

**Sigma:** S1250

>>Variant: (6 $\alpha$ ,11 $\alpha$ H)-form

**Synonym(s):**  $\beta$ -Santonin

**CAS Registry Number:** 481-07-2

**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>3</sub>

**Molecular Weight:** 246.305

**Accurate Mass:** 246.125595

**Percentage Composition:** C 73.15%; H 7.37%; O 19.49%

**Biological Source:** Constit. of *Artemisia* spp.

**Physical Description:** Cryst. (EtOH)

**Melting Point:** Mp 216-218°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>14</sup> -137.2 (CHCl<sub>3</sub>)

>>Variant: (6 $\beta$ ,11 $\alpha$ H)-form

**Synonym(s):** 6-Epi- $\beta$ -santonin. Santonin D

**CAS Registry Number:** 1618-77-5

**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>3</sub>

**Molecular Weight:** 246.305

**Accurate Mass:** 246.125595

**Percentage Composition:** C 73.15%; H 7.37%; O 19.49%

**Biological Source:** Constit. of *Artemisia cina*