



Formula: C<sub>15</sub>H<sub>18</sub>O<sub>4</sub>

MW: 262.31

Salt: H<sub>2</sub>O

CAS: 10180-88-8

TNP NUMBER: TNP00249

MDL NUMBER: MFCD06668130

IUPAC: (5S,7S,2R,6R)-7-hydroxy-5,9,13-trimethyl-3-oxatricyclo[8.3.0.0]trideca-9,12-diene-4,11-dione

Smiles: C1C(=C2C(C=C(C2[C@@H]2[C@@H]([C@H]1O)[C@H](C)C(=O)O2)C)=O)C

THERAPEUTIC CATEGORY: a hypolipidemic, antiatherosclerotic, anti-inflammatory agent, with angioprotective and hepatoprotective activity; antiulcerous.

REFERENCE: # Rybalko, J. Gen. Chem. (1963) (Russian). 33(8):2734 # Syrov et al., Chem. Pharm. J. (1991) (Russian). 2:42-45

SOURCE: Sesquiterpene lactone C<sub>15</sub>H<sub>18</sub>O<sub>4</sub>.H<sub>2</sub>O from plants of the Compositae family.

ACCEPTORS: 4

DONORS: 1

ROTATION BONDS: 0

N+O: 4

Chiral Centers: 5

LogP: 2.7

LogS: -3.91

LIPINSKI: 4

Synonyms: AUSTRICINE

CAS:

MF:C14H16O4

MW:248.27

EINECS:

Product Categories: AUSTRICINE

Chemical Properties: storage temp. 2-8C

Safety Information: Safety Statements 22-24/25 AUSTRICINE

Usage And Synthesis: AUSTRICINE

