



Formula: C₁₅H₁₈O₃

MW: 246.31

CAS: 481-06-1

MDL: MFCD05618264

TNP: TNP00095

SANTONIN; SANTONIN, A-; (-)-Santonine;
[3S-(3 α ,3 α ,5 β ,9 β)]-3 α ,5,5 α ,9 β -Tetrahydro-3,5 α ,9-trimethylnaphtho[1,2-b]furan
-2,8(3H,4H)dione; 1,2,3,4,4 α ,7-Hexahydro-1-hydroxy-alpha,
4 α ,8-trimethyl-7-oxo-2-naphthaleneacetic acid gamma-lactone; 11-Epiiso



LogP: -1.27

LogS: -3.18

Acceptors: 3

Donors: 0

Rotation Bonds: 0

Chiral Centers: 4

N+O: 3

LIPINSKY: 4

IUPAC: (2S,5S,6S,9S)-5,9,13-trimethyl-3-oxatricyclo[7.4.0.0]trideca-1(13),10-diene-4,12-dione

Smiles: C=12C3OC(=O)C(C3CC[C]2(C=CC(C1C)=O)C)C

Specification: Miscellaneous Natural Products SANTONIN Chemical Properties:

mp 172-173 C(lit.) refractive index -172.5 (C=2, CHCl₃) storage temp. 2-8C Merck 8361 CAS
DataBase Reference 481-06-1 (CAS DataBase Reference) Safety Information Hazard Codes Xn
Risk Statements 22 Safety Statements 22-24/25 RIDADR 2811 WGK Germany 3 RTECS
LE3150000 HazardClass 6.1(a) PackingGroup II SANTONIN Usage And Synthesis
SANTONIN