



Formula: C₁₇H₂₆O₄

MW: 294.39

CAS: 550-24-3

MDL: MFCD00016369

TNP: TNP00137

2,5-dihydroxy-3-undecyl-p-benzoquinon; 4-dione,2,5-dihydroxy-3-undecyl-5-cyclohexadiene-1;
embelicacid; emberine; APOPTOSIS ACTIVATOR III; EMBELIN;
2,5-DIHYDROXY-3-UNDECYL-1,4-BENZOQUINONE;
2,5-DIHYDROXY-3-UNDECYL-2,5-CYCLOHEXADIENE-1,4-DIONE



LogP: 4.69

LogS: -5.19

Acceptors: 4

Donors: 2

Rotation Bonds: 12

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

IUPAC: 2,5-dihydroxy-3-undecylcyclohexa-2,5-diene-1,4-dione

Smiles: C1(=C(C(C=C(C1=O)O)=O)O)CCCCCCCCCCC

Specification: Anthraquinones, Hydroquinones and Quinones; Caspases/Apoptosis EMBELIN

Chemical Properties:

mp 142-143C storage temp. Store at +4C solubility DMSO: >10 mg/mL form solid Safety Information WGK Germany 3 RTECS DK4230000 EMBELIN Usage And Synthesis Biological ActivityCell-permeable, non-peptide inhibitor of X-linked inhibitor of apoptosis (XIAP) (IC 50 = 4.1