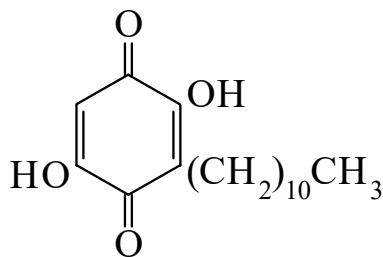




>>Entry Name: **2,5-Dihydroxy-3-undecyl-1,4-benzoquinone**

Synonym(s): 2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione, 9CI. **Embelin**. Embelic acid. Embeliaquinone



CAS Registry Number: 550-24-3

Type of Compound Code(s): PA5010 PS8300 XA3300 XA0900 VA7300 VG0320 PA0070

Molecular Formula: C₁₇H₂₆O₄

Molecular Weight: 294.39

Accurate Mass: 294.18311

Percentage Composition: C 69.36%; H 8.90%; O 21.74%

Biological Source: Constit. of *Embelia ribes*, *Embelia tsjersium-cottam*, *Ardisia humilis*, *Rapanea umbellata* and *Connarus ritchiei*. Also from *Embelia robusta*, *Embelia kilimandscharica*, *Myrsine africana*, *Myrsine semiserrata*, *Myrsine capitellata*, *Rapanea neurophylla* and *Embelia barbeyana*

Use/Importance: Anthelmintic, potent oral contraceptive. Used as a 1% soln. in EtOH for photometric detn. of Al, Be, Ba, Ca, Mg, Sr, Th, U

Physical Description: Orange cryst. (MeOH or hexane/EtOH)

Melting Point: Mp 145-146°

Solubility: Insol. H₂O

Calculated Log P Data: Log P 5.14 (calc)

UV: [base] λ_{max} (solvent not reported) (Derep) [neutral] λ_{max} 292 (ε 16200); 424 (ε 280) (95% EtOH) (Derep) [neutral] λ_{max} 292 (ε 17400); 426 (ε 340) (MeOH) (Berdy)

Hazard & Toxicity: Exp. reprod. effects (male and female)

Sigma: E2521

>>Derivative: Di-Ac

Molecular Formula: C₂₁H₃₀O₆

Molecular Weight: 378.464

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Yellow cryst. (MeOH aq.)

Melting Point: Mp 54°. Mp 59°

>>Derivative: 5-Me ether

Synonym(s): 2-Hydroxy-5-methoxy-3-undecyl-1,4-benzoquinone. **5-O-Methylembelin**

CAS Registry Number: 56005-10-8

Type of Compound Code(s): VG0320 VA7300

Molecular Formula: C₁₈H₂₈O₄

Molecular Weight: 308.417

Accurate Mass: 308.19876

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Biological Source: Constit. of *Aegiceras corniculatum* and *Myrsine africana*

Use/Importance: Piscicide

Physical Description: Orange cryst.

Melting Point: Mp 95-96°

UV: [base] λ_{max} (solvent not reported) (Derep) [neutral] λ_{max} 285 (ε 398) (95% EtOH) (Derep)

>>Derivative: Di-Me ether

Molecular Formula: C₁₉H₃₀O₄

Molecular Weight: 322.444

Percentage Composition: C 70.77%; H 9.38%; O 19.85%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 58°

References: