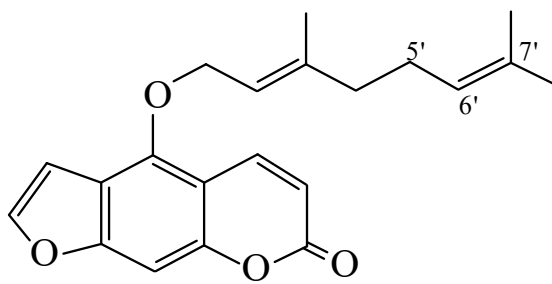




>>Entry Name: Bergamottin

ENTRY UNDER REVIEW

Synonym(s): 4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl. Bergaptol geranyl ether. 5-Geranyloxypsoralen. Bergaptin



CAS Registry Number: 7380-40-7

Molecular Formula: C₂₁H₂₂O₄

Molecular Weight: 338.402

Accurate Mass: 338.15181

Percentage Composition: C 74.54%; H 6.55%; O 18.91%

Biological Source: Constit. of bergamot oil. Also from lemon oil and oils of other *Citrus* spp. and *Daucus carota*

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 59-61° (54°)

>>Derivative: 6',7'-Epoxide

CAS Registry Number: 105866-30-6

Molecular Formula: C₂₁H₂₂O₅

Molecular Weight: 354.402

Accurate Mass: 354.146725

Percentage Composition: C 71.17%; H 6.26%; O 22.57%

Biological Source: Constit. of grapefruit (*Citrus paradisi*) peel oil

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 82.5-83.5°

>>Derivative: 2',3';6',7'-Bisepoxide

Synonym(s): Tortuosin

CAS Registry Number: 89787-38-2

Molecular Formula: C₂₁H₂₂O₆

Molecular Weight: 370.401

Accurate Mass: 370.14164

Percentage Composition: C 68.10%; H 5.99%; O 25.92%

Biological Source: Constit. of *Seseli tortuosum*

Physical Description: Cryst.

Melting Point: Mp 156-157°

>>Derivative: 5'-Hydroxy

Synonym(s): Notopterol

CAS Registry Number: 88206-46-6

Molecular Formula: C₂₁H₂₂O₅

Molecular Weight: 354.402

Accurate Mass: 354.146725

Percentage Composition: C 71.17%; H 6.26%; O 22.57%

Biological Source: Constit. of *Notopterygium incisum*

Use/Importance: Analgesic

Physical Description: Needles (EtOAc/hexane)

Melting Point: Mp 90-92°

Other Data: Opt. inactive