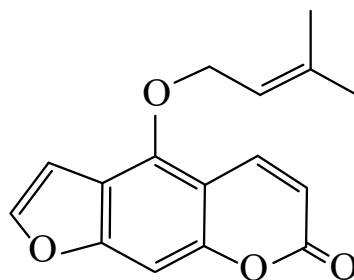




>>Entry Name: Isoimperatorin

Synonym(s): 4-[(3-Methyl-2-butenyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl, 8Cl. 4-Prenyloxypsoralen. Auraptin. Cnidin



CAS Registry Number: 482-45-1

Molecular Formula: C₁₆H₁₄O₄

Molecular Weight: 270.284

Accurate Mass: 270.08921

Percentage Composition: C 71.10%; H 5.22%; O 23.68%

Biological Source: Constit. of *Imperatoria ostruthium* and *Angelica* spp. Also from *Cnidium dubium*. Also in *Peucedanum*, *Prangos*, *Ruta*, *Cachrys* and *Hippomarathrum* spp.

Use/Importance: Has spasmolytic and antineoplastic props.

Melting Point: Mp 109°

Calculated Log P Data: Log P 3.8 (calc)

UV: [neutral] λ_{max} 222 (ε 21700); 250 (ε 16000); 259 (ε 14300); 267 (ε 13900); 310 (ε 12400) (MeOH) [neutral] λ_{max} 222 (ε 21700); 250 (ε 16000); 259 (ε 14300); 267 (ε 13900); 310 (ε 12400) (MeOH) (Berdy) [neutral] λ_{max} 217 (ε 12900); 222 (ε 11250); 251 (ε 4900); 270 (ε 6350); 308 (ε 6880) (EtOH) (Berdy)

References:

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