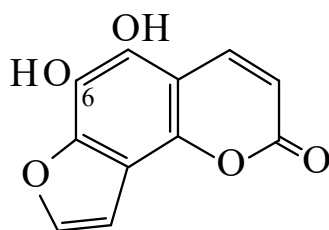




>>Entry Name: 5,6-Dihydroxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9Cl



Molecular Formula: C₁₁H₆O₅

Molecular Weight: 218.165

Accurate Mass: 218.021525

Percentage Composition: C 60.56%; H 2.77%; O 36.67%

>>Derivative: Di-Me ether

Synonym(s): 5,6-Dimethoxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9Cl. **Pimpinellin**

CAS Registry Number: 131-12-4

Molecular Formula: C₁₃H₁₀O₅

Molecular Weight: 246.219

Accurate Mass: 246.052825

Percentage Composition: C 63.42%; H 4.09%; O 32.49%

Biological Source: Constit. of *Pimpinella saxifraga*. Also from *Pimpinella magna* and numerous *Heracleum* spp.

Use/Importance: GABA receptor antagonist, phytoalexin

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 117-119°

>>Derivative: 5-Me ether, 6-*O*-(3-methyl-2-butenyl)

Synonym(s): 6-Isopentenylxyisobergapten

CAS Registry Number: 24099-29-4

Molecular Formula: C₁₇H₁₆O₅

Molecular Weight: 300.31

Accurate Mass: 300.099775

Percentage Composition: C 67.99%; H 5.37%; O 26.64%

Biological Source: From *Angelica genuflexa*

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 95-96°

>>Derivative: 5-Me ether, 6-*O*-(2*R*,3-dihydroxy-3-methylbutanoyl)

Synonym(s): Heraclesol

CAS Registry Number: 67278-85-7

Molecular Formula: C₁₇H₁₈O₇

Molecular Weight: 334.325

Accurate Mass: 334.105255

Percentage Composition: C 61.07%; H 5.43%; O 33.50%

Biological Source: Constit. of *Heracleum leskovii*

Physical Description: Cryst.

Melting Point: Mp 117-118°

Optical Rotation: [α]_D²⁰+30 (MeOH)

References:

Dreyer, D.L., *J.O.C.*, 1970, **35**, 2294-2297, (*Isopentenylxybergapten*)

Komisarenko, N.F. *et al.*, *Khim. Prir. Soedin.*, 1978, **14**, 184-187; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 149-151, (*Heraclesol*)

Reed, M.W. *et al.*, *J.O.C.*, 1988, **53**, 4166-4171, (*synth*)