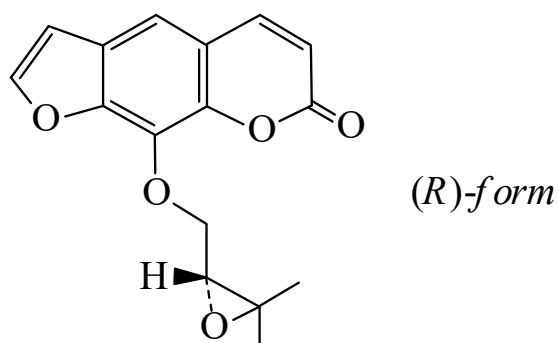




>>Entry Name: Heraclenin

Synonym(s): 9-[(3,3-Dimethyloxiranyl)methoxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl. Imperatorin oxide. Oxyimperatorin. Epoxyimperatorin. Prangenin



Molecular Formula: C₁₆H₁₄O₅

Molecular Weight: 286.284

Accurate Mass: 286.084125

Percentage Composition: C 67.13%; H 4.93%; O 27.94%

Use/Importance: Antiinflammatory agent

Calculated Log P Data: Log P 2.85 (calc)

UV: [neutral] λ_{max} 248 (ε 24500); 262 (ε 12800); 299 (ε 12200) (EtOH) (Berdy)

>>Variant: (*R*)-form

CAS Registry Number: 2880-49-1

Molecular Formula: C₁₆H₁₄O₅

Molecular Weight: 286.284

Accurate Mass: 286.084125

Percentage Composition: C 67.13%; H 4.93%; O 27.94%

Biological Source: Constit. of *Heracleum candicans*, *Citrus trifoliata* and several other spp.

Physical Description: Cryst. (MeOH)

Melting Point: Mp 111°

Optical Rotation: [α]_D³²+22 (Py)

>>Variant: (*S*)-form

CAS Registry Number: 6432-69-5

Molecular Formula: C₁₆H₁₄O₅

Molecular Weight: 286.284

Accurate Mass: 286.084125

Percentage Composition: C 67.13%; H 4.93%; O 27.94%

Biological Source: Constit. of *Phebalium drummondii*

Physical Description: Prisms (CCl₄ or MeOH)

Melting Point: Mp 106.5-108°

Optical Rotation: [α]_D²³-24 (c, 3.19 in Py)

>>Variant: (±)-form

Molecular Formula: C₁₆H₁₄O₅

Molecular Weight: 286.284

Accurate Mass: 286.084125

Percentage Composition: C 67.13%; H 4.93%; O 27.94%

Biological Source: Constit. of another strain of *Phebalium drummondii*

Melting Point: Mp 113-114.5°

References:

Kidwai, A.R. *et al.*, *Tetrahedron*, 1964, **20**, 87, (*isol, struct*)

Chow, P.W. *et al.*, *Aust. J. Chem.*, 1966, **19**, 483, (*isol*)

Lemmich, J. *et al.*, *Acta Chem. Scand.*, 1969, **23**, 962, (*abs config*)

Adesogan, G.K. *et al.*, *Phytochemistry*, 1973, **12**, 2310, (*isol*)

Guiotto, A. *et al.*, *Z. Naturforsch., C*, 1973, **28**, 260, (*isol*)

Adityachaudhury, I., *Phytochemistry*, 1974, **13**, 235, (*isol, spectra*)

Sood, S. *et al.*, *J. Indian Chem. Soc.*, 1978, **55**, 850, (*isol*)