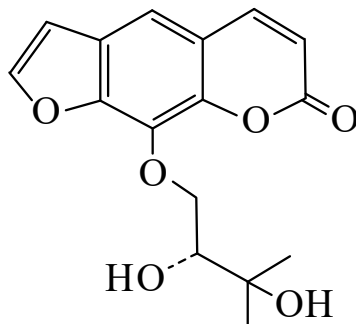




>>Entry Name: Heraclenol

Synonym(s): 9-(2,3-Dihydroxy-3-methylbutoxy)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl. Isosaxalin. Komalin. Prangenin hydrate. Heraclenin hydrate



CAS Registry Number: 2817-09-6

Related CAS Registry Numbers(s): 31575-93-6

Extra CAS Registry Numbers(s): 118407-74-2

Molecular Formula: C₁₆H₁₆O₆

Molecular Weight: 304.299

Accurate Mass: 304.09469

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

>>Variant: (*R*)-form

CAS Registry Number: 26091-76-9

Molecular Formula: C₁₆H₁₆O₆

Molecular Weight: 304.299

Accurate Mass: 304.09469

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Biological Source: Obt. from roots of *Angelica* and *Heracleum* spp.

Melting Point: Mp 117-118°

Optical Rotation: $[\alpha]_D^{32} +16.5$ (Py)

>>Derivative: 3'-*O*-β-D-Glucopyranoside

CAS Registry Number: 32207-10-6

Molecular Formula: C₂₂H₂₆O₁₁

Molecular Weight: 466.441

Accurate Mass: 466.147515

Percentage Composition: C 56.65%; H 5.62%; O 37.73%

Biological Source: Isol. from roots of *Heracleum candicans*

Melting Point: Mp 198°

Optical Rotation: $[\alpha]_D^{25} +9$ (H₂O)

>>Derivative: 2'-*O*-Ac

CAS Registry Number: 49586-43-8

Extra CAS Registry Numbers(s): 132341-07-2

Biological Source: Constit. of *Ammi majus*

Melting Point: Mp 101-102° (95-96°)

Other Data: Abs. config. of nat. prod. not specifically reported. Mp identical with semisynthetic *R*-form prev. known

>>Derivative: 2',3'-Di-Ac

Molecular Formula: C₂₀H₂₀O₈

Molecular Weight: 388.373

Accurate Mass: 388.11582

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Melting Point: Mp 65°. Mp 98-100°