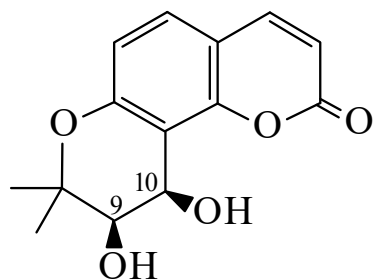




>>Entry Name: Khellactone

Synonym(s): 9,10-Dihydro-9,10-dihydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b'*]dipyran-2-one, 9Cl. 3',4'-Dihydroxy-3',4'-dihydroseselin



(9*R*,10*R*)-form

CAS Registry Number: 518-76-3

Related CAS Registry Numbers(s): 6005-18-1 10182-81-7 15575-57-2 76250-53-8

Molecular Formula: C<sub>14</sub>H<sub>14</sub>O<sub>5</sub>

Molecular Weight: 262.262

Accurate Mass: 262.084125

Percentage Composition: C 64.12%; H 5.38%; O 30.50%

>>Variant: (9*R*,10*R*)-form

Synonym(s): (+)-*cis*-form

CAS Registry Number: 24144-61-4

Molecular Formula: C<sub>14</sub>H<sub>14</sub>O<sub>5</sub>

Molecular Weight: 262.262

Accurate Mass: 262.084125

Percentage Composition: C 64.12%; H 5.38%; O 30.50%

Biological Source: Isol. from *Seseli gummiferum*

Physical Description: Cryst. (C<sub>6</sub>H<sub>6</sub>/petrol)

Melting Point: Mp 174-175°

Optical Rotation: [α]<sub>D</sub><sup>22</sup>+104 (c, 0.864 in EtOH). [α]<sub>D</sub><sup>20</sup>+80.9 (c, 1.041 in CHCl<sub>3</sub>)

>>Derivative: 9-*O*-Sulfate

CAS Registry Number: 92142-33-1

Molecular Formula: C<sub>14</sub>H<sub>14</sub>O<sub>8</sub>S

Molecular Weight: 342.326

Accurate Mass: 342.04094

Percentage Composition: C 49.12%; H 4.12%; O 37.39%; S 9.37%

Biological Source: Constit. of *Seseli libanotis*

Physical Description: Non-cryst. (as K salt)

Optical Rotation: [α]<sub>D</sub><sup>23</sup>−51 (c, 0.3 in MeOH)

Other Data: CAS no. refers to K salt

>>Derivative: 9-*O*-β-D-Glucopyranoside

Synonym(s): Campestrinoside. Praeroside II

CAS Registry Number: 84458-87-7

Molecular Formula: C<sub>20</sub>H<sub>24</sub>O<sub>10</sub>

Molecular Weight: 424.404

Accurate Mass: 424.13695

Percentage Composition: C 56.60%; H 5.70%; O 37.70%

Biological Source: Constit. of *Seseli campestre* and *Peucedanum praeruptorum*

Melting Point: Mp 172-173°

Optical Rotation: [α]<sub>D</sub>−272.5 (EtOH)

>>Derivative: Di-Ac

Molecular Formula: C<sub>18</sub>H<sub>18</sub>O<sub>7</sub>

Molecular Weight: 346.336

Accurate Mass: 346.105255

Percentage Composition: C 62.42%; H 5.24%; O 32.34%

Physical Description: Cryst. (Me<sub>2</sub>CO aq.)

Melting Point: Mp 132-134°

Optical Rotation: [α]<sub>D</sub><sup>24</sup>−17.4 (c, 0.743 in CHCl<sub>3</sub>)