



Optical Rotation: $[\alpha]_{\text{D}} +36$ (CHCl_3)

>>**Variant:** (S)-form

CAS Registry Number: 139079-42-8

Molecular Formula: $\text{C}_{16}\text{H}_{16}\text{O}_6$

Molecular Weight: 304.299

Accurate Mass: 304.09469

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

Physical Description: Constit. of *Esenbeckia grandiflora* ssp. *grandiflora*, *Magydaris pastinacea* and *Skimmia japonica*

Melting Point: Mp 115-116°

Optical Rotation: $[\alpha]_{\text{D}} -15$ (c, 0.7 in Py)

>>**Variant:** (±)-form

Molecular Formula: $\text{C}_{16}\text{H}_{16}\text{O}_6$

Molecular Weight: 304.299

Accurate Mass: 304.09469

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

Biological Source: Isol. from *Prangos pabularia* and *Prangos serawschanica*

Physical Description: Cryst. (Et_2O /petrol)

Melting Point: Mp 128-129°

>>**Variant:** (ξ)-form

Molecular Formula: $\text{C}_{16}\text{H}_{16}\text{O}_6$

Molecular Weight: 304.299

Accurate Mass: 304.09469

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

>>**Derivative:** 2'-(2-Hydroxypropanoyl)

Synonym(s): Fesumtuorin B

Molecular Formula: $\text{C}_{19}\text{H}_{20}\text{O}_8$

Molecular Weight: 376.362

Accurate Mass: 376.11582

Percentage Composition: C 60.64%; H 5.36%; O 34.01%

Biological Source: Cosntit. of the dried roots of *Ferula sembul*

Optical Rotation: $[\alpha]_{\text{D}}^{25} +3.6$ (c, 0.4 in MeOH)

UV: [neutral] λ_{max} 217 (log ϵ 4.28); 248 (log ϵ 4.18); 299 (log ϵ 3.91) (MeOH)

Other Data: Stereochem. not determined

References:

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Sharma, Y.N. *et al.*, *Naturwissenschaften*, 1964, **51**, 537, (*isol*)
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Bandopadhyay, M. *et al.*, *Indian J. Chem.*, 1970, **8**, 855; 1146; 1973, **11**, 530, (*isol, synth*)
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Ivie, G.W. *et al.*, *J. Agric. Food Chem.*, 1978, **26**, 1394, (*isol*)
Razdan, T.K. *et al.*, *Phytochemistry*, 1982, **21**, 923, (*isol, ir, uv, pmr, ms*)
Harkar, S. *et al.*, *Phytochemistry*, 1984, **23**, 419, (*isol, ir, ms*)
Sun, H. *et al.*, *Pharmazie*, 1986, **41**, 888
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Zhou, P. *et al.*, *Phytochemistry*, 2000, **53**, 689-697, (*Fesumtuorin B*)