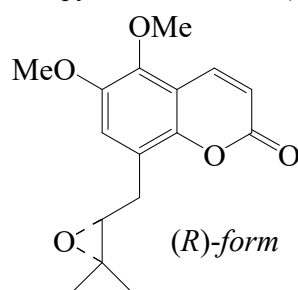




>>Entry Name: Sibiricin

Synonym(s): 8-[(3,3-Dimethyloxiranyl)methyl]-5,7-dimethoxy-2*H*-1-benzopyran-2-one, 9Cl. 8-(2,3-Epoxy-3-methylbutyl)-5,7-dimethoxycoumarin. Isoaculeatin



Molecular Formula: C₁₆H₁₈O₅

Molecular Weight: 290.315

Accurate Mass: 290.115425

Percentage Composition: C 66.20%; H 6.25%; O 27.56%

>>Variant: (R)-form

CAS Registry Number: 18196-01-5

Molecular Formula: C₁₆H₁₈O₅

Molecular Weight: 290.315

Accurate Mass: 290.115425

Percentage Composition: C 66.20%; H 6.25%; O 27.56%

Biological Source: Isol. from *Seseli sibiricum* and *Libanotis buchtormensis*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 152-153°

Optical Rotation: [α]_D³⁰+60.4 (dioxan)

>>Variant: (S)-form

CAS Registry Number: 95188-34-4

Molecular Formula: C₁₆H₁₈O₅

Molecular Weight: 290.315

Accurate Mass: 290.115425

Percentage Composition: C 66.20%; H 6.25%; O 27.56%

Biological Source: Constit. of *Murraya gleinei*

Physical Description: Needles (CHCl₃/petrol)

Melting Point: Mp 148-149°

Optical Rotation: [α]_D²⁵-59.7 (CHCl₃)

References:

Bohlmann, F. *et al.*, *Chem. Ber.*, 1968, **101**, 2741, (*isol*)

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González, A.G. *et al.*, *An. Quim.*, 1973, **69**, 1013, (*isol*)

Chang, C. *et al.*, *J.O.C.*, 1977, **42**, 1337, (*nmr*)

Wickramaratne, D.B.M. *et al.*, *Phytochemistry*, 1984, **23**, 2964

Wazeer, M.I.M. *et al.*, *Can. J. Spectrosc.*, 1990, **35**, 57, (*cmr*)

Kinoshita, T. *et al.*, *Chem. Pharm. Bull.*, 1996, **44**, 1208, (*isol, cmr, abs config*)