



Molecular Formula: C₁₂H₁₈O₅

Molecular Weight: 242.271

Accurate Mass: 242.115425

Percentage Composition: C 59.49%; H 7.49%; O 33.02%

Biological Source: Constit. of *Acorus tatarinowii*

Other Data: Isol. as a mixture of *erythro*- and *threo*-isomers

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

Synonym(s): β-Asarone

CAS Registry Number: 5273-86-9

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Biological Source: Constit. of *Acorus* spp.

Boiling Point: Bp₁₂ 162-163°

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O

UV: [neutral] λ_{max} 208 (); 250 (); 300 () (MeOH) (Berdy)

Aldrich: 22107-4

Sigma: A6654

>>**Derivative:** Picrate

Physical Description: Brownish-black needles

Melting Point: Mp 82°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1054D, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 209C; 210A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 981C; 987B, (*ir*)

Eggers, F. *et al.*, *Ber.*, 1899, **32**, 290, (*synth*)

Baxter, R.M., *Can. J. Chem.*, 1962, **40**, 154, (*config*)

Patra, A. *et al.*, *J. Nat. Prod.*, 1981, **44**, 668, (*cmr*)

Mulzer, J. *et al.*, *Angew. Chem., Int. Ed.*, 1983, **22**, 628, (*synth*)

Della Greca, M. *et al.*, *Phytochemistry*, 1989, **28**, 2319-2321, (*epoxide*)

Diaz, F. *et al.*, *Org. Prep. Proced. Int.*, 1991, **23**, 133, (*synth, bibl*)

Nawamaki, K. *et al.*, *Phytochemistry*, 1996, **43**, 1175, (*isol, pmr*)

Gonzalez, M.C. *et al.*, *Phytochemistry*, 1996, **43**, 1361, (*isol, uv, ir, pmr, cmr, ms*)

Siergiejczyk, L. *et al.*, *Magn. Reson. Chem.*, 2000, **38**, 1037-1038, (*pmr, cmr*)

Hu, J. *et al.*, *Planta Med.*, 2000, **66**, 662-664, (*cis-Epoxyasarone, Dihydroxyasarone*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, IHX400