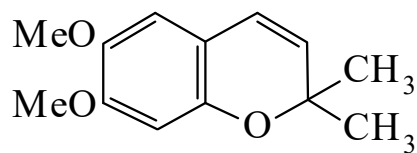




>>Entry Name: 6,7-Dimethoxy-2,2-dimethyl-2H-1-benzopyran, 9Cl

Synonym(s): 6,7-Dimethoxy-2,2-dimethyl-3-chromene. Ageratochromene. Precocene II



CAS Registry Number: 644-06-4

Type of Compound Code(s): VI0030

Molecular Formula: C₁₃H₁₆O₃

Molecular Weight: 220.268

Accurate Mass: 220.109945

Percentage Composition: C 70.89%; H 7.32%; O 21.79%

Biological Source: From *Ageratum houstonianum*, *Ageratum conyzoides*, *Ageratum mexicanum* and *Verbesina* spp.

Use/Importance: Antiallotropin (induces premature ecdysis in insects)

Physical Description: Pale-yellow needles (MeOH) or oil

Melting Point: Mp 49-50°

Boiling Point: Bp₄ 145-150°

Hazard & Toxicity: Exp. carcinogenic data

Aldrich: 19491-3

Sigma: D2263

>>Derivative: O⁷-De-Me, O⁷-Et

Synonym(s): 7-Ethoxy-6-methoxy-2,2-dimethyl-2H-1-benzopyran. Precocene III. 7-Ethoxyprecocene II

CAS Registry Number: 65383-73-5

Molecular Formula: C₁₄H₁₈O₃

Molecular Weight: 234.294

Accurate Mass: 234.125595

Percentage Composition: C 71.77%; H 7.74%; O 20.49%

Source/Synthesis: Synthetic

Use/Importance: Proallatocidin; the most potent precocene analogue having =10 times the activity of Precocene II

Physical Description: Oil

Boiling Point: Bp_{0.1} 109°

Refractive Index: n_D²⁰ 1.5560

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 1063A, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 227A, (*nmr*)
Hlubucek, J.R. *et al.*, *Aust. J. Chem.*, 1971, **24**, 2347, (*synth*)
Kasturi, T.R. *et al.*, *Indian J. Chem.*, 1973, **11**, 91, (*isol*)
Suga, T. *et al.*, *Phytochemistry*, 1975, **14**, 306, (*isol*, *ir*, *uv*, *pmr*)
Bowers, W.S. *et al.*, *Science (Washington, D.C.)*, 1976, **193**, 542, (*isol*, *synth*, *use*)
Ohta, T. *et al.*, *Chem. Pharm. Bull.*, 1977, **28**, 2788, (*synth*)
Ohta, T. *et al.*, *J. Agric. Food Chem.*, 1977, **25**, 478, (*metab*)
Schwartz, M., *J. Het. Chem.*, 1977, **14**, 333, (*synth*)
Bohlmann, F. *et al.*, *Chem. Ber.*, 1978, **111**, 263, (*isol*)
Kiehlmann, E. *et al.*, *Org. Prep. Proced. Int.*, 1982, **14**, 337, (*Precocene III*)
Teixidor, P. *et al.*, *Heterocycles*, 1988, **27**, 2459, (*synth*)
Timár, T. *et al.*, *J. Het. Chem.*, 1988, **25**, 871, (*synth*, *pmr*, *cmr*, *ms*, *bibl*)
Pandey, G. *et al.*, *J.O.C.*, 1988, **53**, 2364, (*synth*)
Baruah, R.N., *Chem. Ind. (London)*, 1989, 725, (*synth*)
Timar, T. *et al.*, *Magn. Reson. Chem.*, 1989, **27**, 303, (*cmr*)
Siebertz, R. *et al.*, *Phytochemistry*, 1990, **29**, 2135, (*biosynth*)
Miranda, M.A. *et al.*, *Heterocycles*, 1991, **32**, 1159-1166, (*synth*, *Precocene III*)
Kulkarni, S.A. *et al.*, *Synth. Commun.*, 1992, **22**, 1555, (*synth*)
Bissada, S. *et al.*, *Can. J. Chem.*, 1994, **72**, 1866, (*synth*, *pmr*)
Steinbeck, C. *et al.*, *J. Nat. Prod.*, 1997, **60**, 627, (*isol*, *pmr*, *cmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AEX850