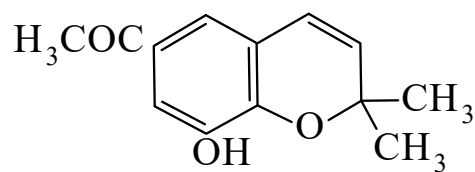




>>Entry Name: 6-Acetyl-8-hydroxy-2,2-dimethyl-2H-1-benzopyran

Synonym(s): 6-Acetyl-8-hydroxy-2,2-dimethyl-3-chromene



CAS Registry Number: 67667-62-3

Molecular Formula: C₁₃H₁₄O₃

Molecular Weight: 218.252

Accurate Mass: 218.094295

Percentage Composition: C 71.54%; H 6.47%; O 21.99%

Biological Source: Constit. of *Iostephane* sp., *Isocarpha* sp., *Lagascea* sp., *Simsia* sp. and *Viguiera* sp.

Use/Importance: Antioxidant

Physical Description: Cryst.

Melting Point: Mp 135-137°

>>Derivative: Me ether

Synonym(s): 6-Acetyl-8-methoxy-2,2-dimethyl-2H-1-benzopyran. 6-Acetyl-8-methoxy-2,2-dimethyl-2H-chromene. **Acetovanillochromene**

CAS Registry Number: 34155-83-4

Molecular Formula: C₁₄H₁₆O₃

Molecular Weight: 232.279

Accurate Mass: 232.109945

Percentage Composition: C 72.39%; H 6.94%; O 20.66%

Biological Source: Constit. of *Ageratina scorodonioides* and *Eupatorium riparium*

Physical Description: Cryst. (hexane)

Melting Point: Mp 73-73.5°

>>Derivative: 5-Hydroxy, 8-Me ether

Synonym(s): 6-Acetyl-5-hydroxy-8-methoxy-2,2-dimethyl-2H-1-benzopyran

CAS Registry Number: 61670-29-9

Molecular Formula: C₁₄H₁₆O₄

Molecular Weight: 248.278

Accurate Mass: 248.10486

Percentage Composition: C 67.73%; H 6.50%; O 25.78%

Biological Source: Isol. from *Flourensia cernua* and *Ageratina* spp.

Physical Description: Needles (Et₂O/petrol)

Melting Point: Mp 88°

>>Derivative: 5-Methoxy, 8-Me ether

Synonym(s): 6-Acetyl-5,8-dimethoxy-2,2-dimethyl-2H-1-benzopyran

CAS Registry Number: 62458-48-4

Molecular Formula: C₁₅H₁₈O₄

Molecular Weight: 262.305

Accurate Mass: 262.12051

Percentage Composition: C 68.69%; H 6.92%; O 24.40%

Biological Source: Constit. of *Ageratina scorodonioides*

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 63°

References:

- Taylor, D.R. *et al.*, *Phytochemistry*, 1971, **10**, 1665, (*isol*)
Bohlmann, F. *et al.*, *Chem. Ber.*, 1977, **110**, 295; 301, (*isol*)
Bohlmann, F. *et al.*, *Phytochemistry*, 1978, **17**, 566, (*isol*)
Bohlmann, F. *et al.*, *Annalen*, 1980, 185, (*synth*)
Ahluwalia, V.K. *et al.*, *Indian J. Chem., Sect. B*, 1982, **21**, 1039, (*synth*)
Tsuda, H. *et al.*, *Heterocycles*, 1997, **44**, 139, (*synth, pmr*)