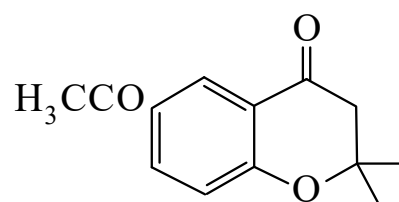




>>Entry Name: 6-Acetyl-2,3-dihydro-2,2-dimethyl-4*H*-1-benzopyran-4-one, 9Cl

Synonym(s): 6-Acetyl-2,2-dimethyl-4-chromanone



CAS Registry Number: 68799-41-7

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 *Ambrosia cumanensis* and *Gnoxys psilophylla*

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 96°

>>Derivative: 1'-Hydroxy

Synonym(s): 6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-2-methyl-4*H*-1-benzopyran-4-one. 6-Acetyl-2-hydroxymethyl-2-methyl-4-chromanone

Molecular Formula: C₁₃H₁₄O₄

Molecular Weight: 234.251

Accurate Mass: 234.08921

Percentage Composition: C 66.66%; H 6.02%; O 27.32%

Biological Source: Constit. of *Gynura formosana*

Physical Description: Pale yellow solid

Melting Point: Mp 79-80°

Optical Rotation: [α]_D +11.4

UV: [neutral] λ_{max} 240 (log ε 4); 271 (log ε 3.7); 312 (sh) (); 320 (log ε 3) (no solvent reported)

References:

Bohlmann, F. *et al.*, *Phytochemistry*, 1977, **16**, 575; 1979, **18**, 339, (*isol*)

Bohlmann, F. *et al.*, *Chem. Ber.*, 1981, **114**, 147, (*synth*)

Jong, T.-T. *et al.*, *Phytochemistry*, 1997, **44**, 553, (*isol, deriv, uv, pmr, cmr*)