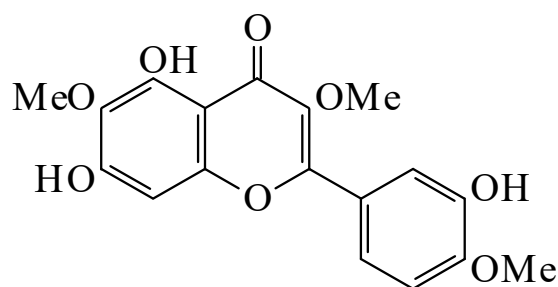




>>Entry Name: 3',5,7-Trihydroxy-3,4',6-trimethoxyflavone

Synonym(s): 5,7-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6-dimethoxy-4*H*-1-benzopyran-4-one, 9Cl. **Centaureidin**



CAS Registry Number: 17313-52-9

Molecular Formula: C₁₈H₁₆O₈

Molecular Weight: 360.32

Accurate Mass: 360.08452

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Biological Source: Isol. from *Brickellia laciniata* and many others in the Asteraceae

Use/Importance: Antineoplastic agent

Physical Description: Yellow needles (MeOH)

Melting Point: Mp 196°

Calculated Log P Data: Log P 0.47 (calc)

UV: [neutral] λ_{max} 253 (); 346 () (MeOH) (Berdy) [neutral] λ_{max} 258 (ε 15000); 354 (ε 20000) (EtOH) (Berdy) [base] λ_{max} 265 (); 400 () (MeOH-NAOH) (Berdy)

>>Derivative: 7-*O*-β-D-Glucopyranoside

Synonym(s): **Centaurein**

CAS Registry Number: 35595-03-0

Molecular Formula: C₂₄H₂₆O₁₃

Molecular Weight: 522.462

Accurate Mass: 522.137345

Percentage Composition: C 55.17%; H 5.02%; O 39.81%

Biological Source: Constit. of the root of *Centaurea jacea*. Also from *Brickellia* spp., *Galinsoga* spp. and *Tetragonotheca* spp.

Physical Description: Yellow cryst. + H₂O

Melting Point: Mp 208-209°

Optical Rotation: [α]_D²⁰ -76.6 (c, 1.4 in MeOH)

UV: [neutral] λ_{max} 258 (ε 29420); 349 (ε 29000) (MeOH) (Berdy)

References:

- Farkas, L. *et al.*, *Chem. Ber.*, 1964, **97**, 610; 1666, (*isol, struct*)
Horie, T., *Bull. Chem. Soc. Jpn.*, 1969, **42**, 2701, (*synth*)
Rodriguez, E. *et al.*, *Phytochemistry*, 1972, **11**, 409, (*pmr*)
Timmerman, B.N. *et al.*, *Phytochemistry*, 1979, **18**, 1855
Voirin, B., *Phytochemistry*, 1983, **22**, 2107, (*uv*)