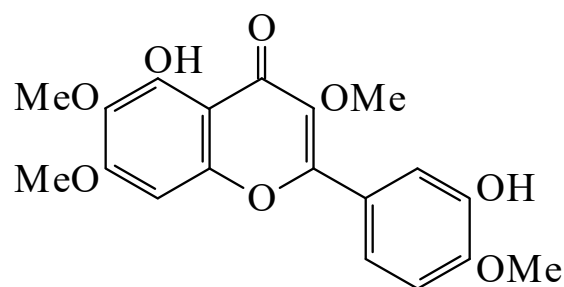




>>Entry Name: 3',5-Dihydroxy-3,4',6,7-tetramethoxyflavone

Synonym(s): 5-Hydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6,7-trimethoxy-4*H*-benzopyran-4-one, 9Cl. **Casticin**. Vitexicarpin



CAS Registry Number: 479-91-4

Type of Compound Code(s): VK5260

Molecular Formula: C₁₉H₁₈O₈

Molecular Weight: 374.346

Accurate Mass: 374.10017

Percentage Composition: C 60.96%; H 4.85%; O 34.19%

Biological Source: Constit. of *Vitex agnus-castus* seeds, other *Vitex* spp., *Brickellia* spp., *Parthenium* spp., *Artemisia lanata*, *Artemisia annua* and others

Physical Description: Prisms (C₆H₆/petrol)

Melting Point: Mp 178-180° (170-172°). Mp 186-187°. Mp 214°

UV: [base] λ_{max} 233 (sh) (ε 11500); 268 (ε 14800); 335 (ε 6760); 375 (ε 5750) (MeOH/NaOH) (Derep) [neutral] λ_{max} 257 (ε 10200); 267 (sh) (ε 8710); 347 (ε 11000) (MeOH) (Derep)

Other Data: Originally thought to be 3,5-Dihydroxy-3',4',7,8-tetramethoxyflavone. Struct. revised in 1989

>>Derivative: 3'-*O*-β-D-Glucopyranoside

CAS Registry Number: 71827-14-0

Type of Compound Code(s): VK5260

Molecular Formula: C₂₅H₂₈O₁₃

Molecular Weight: 536.488

Accurate Mass: 536.152995

Percentage Composition: C 55.97%; H 5.26%; O 38.77%

Biological Source: Isol. from *Chrysosplenium americanum*

Physical Description: Pale yellow needles (MeOH aq.)

Melting Point: Mp 179-183°

References:

- Beliš, I. *et al.*, *J.C.S.*, 1961, 2523
Hörhammer, L. *et al.*, *Tet. Lett.*, 1964, 323, (*struct*)
Hansel, R. *et al.*, *Phytochemistry*, 1965, **4**, 19, (*isol*)
Djermanović, M. *et al.*, *Phytochemistry*, 1975, **14**, 1873, (*isol, uv, ms, pmr*)
Rodriguez, E., *Biochem. Syst. Ecol.*, 1977, **5**, 207, (*isol*)
Iinuma, M. *et al.*, *Chem. Pharm. Bull.*, 1980, **28**, 708, (*cmr*)
Collins, F.W. *et al.*, *Z. Naturforsch., C*, 1981, **36**, 730, (*uv, pmr, ms, glycoside*)
Voirin, B., *Phytochemistry*, 1983, **22**, 2107, (*uv*)
Esteban, M.D. *et al.*, *Phytochemistry*, 1986, **25**, 1502, (*isol*)

Horie, T. *et al.*, *Phytochemistry*, 1989, **28**, 2869, (*isol, struct*)