



Formula: C₁₅H₁₆O₅

MW: 276.29

CAS: 77369-04-1

MDL: MFCD10039710

TNP:

3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-6-methoxy-2H-1-benzopyran-2-one; Obtusidin



LogP: 4.51

LogS: -5.1

Acceptors: 5

Donors: 1

Rotation Bonds: 6

Chiral Centers: 0

N+O: 5

LIPINSKY: 4

IUPAC: 7-((2Z)-4-hydroxy-3-methylbut-2-enyloxy)-6-methoxychromen-2-one

Smiles: c1c(OCC=C(C)CO)c(OC)cc2c1oc(cc2)=O

REFERENCE: Chemistry of Natural Compounds (1983) 18:157-160, March 01, 1983 By Matkarimov, A. D.; Batirov, E. Kh.; Malikov, V. M.; Seitmuratov, E. Show all (4)

SOURCE: The epigeal part of *Haplophyllum obtusifolium* Ledeb has yielded scopoletin and the

following new coumarins: obtusidin, C₁₅H₁₆O₅

Specification: 3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-6-methoxy-2H-1-benzopyran-2-one

3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-6-methoxy-2H-1-benzopyran-2-one Usage And
Synthesis 3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-6-methoxy-2H-1-benzopyran-2-one