



Formula: C₉H₆O₄

MW: 178.14

CAS: 305-01-1

MDL: MFCD00006874

TNP: TNP00643

CICHORIGENIN; CICHERINGENIN; ESCULETOL; ESCULETIN; LABOTEST-BB LT00233229; AESCULETIN; AKOS 215-98; 6,7-DIHYDROXY-CHROMEN-2-ONE



LogP: 3.65

LogS: -3.95

Acceptors: 4

Donors: 2

Rotation Bonds: 2

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

Info: Esculetin 98%

IUPAC: 6,7-dihydroxychromen-2-one

Smiles: c12c(oc(=O)cc1)cc(c(c2)O)O

THERAPEUTIC CATEGORY: Bacteriostatic and antifungal activity

SOURCE: Relatively Widespread among angiosperm families: e.g., in the seeds of Euphorbia lathyris (Euphorbiaceae, in the bark of Fraxinus spp.

Specification: Coumarins; Analytical Chemistry; Mass Spectrometry; Matrix Materials (MALDI-TOF-MS) Esculetin Chemical Properties:

mp 271-273 C(lit.) Water Solubility slightly soluble Merck 14,3697 BRN 152788 CAS DataBase Reference305-01-1(CAS DataBase Reference) NIST Chemistry ReferenceCoumarin, 6,7-dihydroxy-(305-01-1) EPA Substance Registry System2H-1-Benzopyran- 2-one, 6,7-dihydroxy-(305-01-1) Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 26-36-37/39 WGK Germany 3 RTECS GN6382500 6,7-Dihydroxycoumarin English Esculetin Usage And Synthesis Chemical Properties:

YELLOWISH CRYSTALLINE POWDER Esculetin Preparation ProductsSCOPARONE Raw materials1,4-Benzoquinone

Merck 13 Reference: Monograph Number: 0003731

Title: Esculetin

CAS Registry Number: 305-01-1

CAS Name: 6,7-Dihydroxy-2H-1-benzopyran-2-one

Additional Names: 6,7-dihydroxycoumarin; cichorigenin

Molecular Formula: C₉H₆O₄

Molecular Weight: 178.14.

Percent Composition: C 60.68%, H 3.39%, O 35.93%

Literature References: The aglucon of esculin and of cichoriin. By hydrolysis of esculin or of cichoriin: Merz, Arch. Pharm. 270, 486 (1932). By synthesis: Gattermann, K