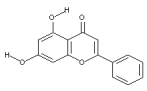

Formula: C15H10O4

MW: 254.24

CAS: 480-40-0

MDL: MFCD00006834

TNP: TNP00395

AKOS NCG1-0026; 5,7-DIHYDROXYFLAVONE;
5,7-dihydroxy-2-phenyl-4h-benzo[b]pyran-4-one;
5,7-DIHYDROXY-2-PHENYL-CHROMEN-4-ONE; LABOTEST-BB LT00440772; CHRYSIN;
CHRYSINE; 5,7-dihydroxy-2-phenyl-4h-1-benzopyran-4-on

LogP: 2.64

LogS: -3.77

Acceptors: 4

Donors: 2

Rotation Bonds: 2

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

Info: Chrysin 99+%

IUPAC: 5,7-dihydroxy-2-phenylchromen-4-one

Smiles: c12c(cc(c3ccccc3)oc1cc(cc2O)O)=O

Specification: Intermediates; FINE Chemical & INTERMEDIATES; Di-substituted Flavones; Biochemistry; Flavonoids Chrysin Chemical Properties:

 mp 284-286 C(lit.) storage temp. 0-6C Merck 14,2256 BRN 233276 Stability:Stable. Incompatible with strong oxidizing agents. CAS DataBase Reference480-40-0(CAS DataBase Reference) Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 22-24/25-36-26 WGK Germany 3 RTECS LK8329050 F 10 5,7-Dihydroxy-2-phenyl-4H-benzo[b]pyran-4-one English Chrysin Usage And Synthesis Chemical Properties:

beige powder Chrysin Raw materialsEthyl acetoacetate-->Benzoyl chloride-->Phloroglucinol dihydrate

Merck 13 Reference: Monograph Number: 0002278

Title: Chrysin

CAS Registry Number: 480-40-0

CAS Name: 5,7-Dihydroxy-2-phenyl-4H-1-benzopyran-4-one

Additional Names: 5,7-dihydroxyflavone; chrysidenon 1438

Molecular Formula: C15H10O4

Molecular Weight: 254.24.

Percent Composition: C 70.86%, H 3.96%, O 25.17%

Literature References: From heartwood of Pinus monticola Dougl., P. excelsa Wall., and P. aristata Engelm., Pinaceae: Linstedt, Acta Chem. Scand. 3, 1147, 1375 (1949); 4, 55 (1950); from bark of Dolichandrone falcata Seem., Bisnomiaceae: Kincl, Naturwissenschaften 42, 646 (1955). Synthesis: Seka, Prosche, Monatsh. Chem. 69, 284 (1936); Hutchins, Wheeler, J. Chem. Soc. 1939, 91; Teoule et al., Bull. Soc. Chim. Fr. 1961, 546.

Properties: Light yellow prisms from methanol, mp 285. uv max: 270, 329 nm (log e 4.40, 3.90). Practically insol in water; sol in alkali hydroxide solns; slightly sol in alcohol, chloroform, ether.

Melting point: mp 285

Absorption maximum: uv max: 270, 329 nm (log e 4.40, 3.90)

Derivative Type: Diacetoxychrysin

Molecular Formula: C19H14O6

Molecular Weight: 338.31.

Percent Composition: C 67.45%, H 4.17%, O 28.38%

Properties: Crystals from ethanol, mp 194-195.

Melting point: mp 194-195

Derivative Type: Methylchrysin

Additional Names: Tectochrysin

Molecular Formula: C16H12O4

Molecular Weight: 268.26.

Percent Composition: C 71.64%, H 4.51%, O 23.86%

Literature References: It is present as such or in the form of a glucoside in buds of Populus spp., Salicaceae. Use of tectochrysin as diuretic: Perrault, US 3155579 (1964 to Laroche Navarron).

Properties: Yellow needles, mp 163. Sol in alcohol, benzene, chloroform.

Melting point: mp 163