



Formula: C<sub>16</sub>H<sub>12</sub>O<sub>6</sub>

MW: 300.27

CAS: 475-25-2

MDL: MFCD00036187

TNP: TNP00288

TIMTEC-BB SBB006464;

2-d]pyran-9(6h)-one,6a,7-dihydro-3,4,6a,10-tetrahydroxy-benz(b)indeno(;

2-d]pyran-9(6h)-one,6a,7-dihydro-3,4,6a,10-tetrahydroxy-benz[b]indeno[;

3,4,6a,10-tetrahydroxy-6a,7-dihydrobenz(b)indeno(1,2-d)pyran-9(6h)-one; abcolhematine[lg;

hemati



LogP: 5.67

LogS: -5.72

Acceptors: 6

Donors: 4

Rotation Bonds: 4

Chiral Centers: 1

N+O: 6

LIPINSKY: 4

IUPAC: 3,4,10,6a-tetrahydroxy-7,6a-dihydroindeno[2,1-c]chroman-9-one

Smiles: C12=C3C(COc4c3ccc(O)c4O)(O)CC1=CC(C(=C2)O)=O

REFERENCE: Merck 13,4651

SOURCE: From logwood

Specification: G-H-I; Stains and Dyes; Stains&Dyes, A to HEMATEIN Chemical Properties:

mp 180 C storage temp. 2-8C Merck 13,4651 Safety 24/25 WGK Germany 3 RTECS DE3120000 F 8-10-23HEMATEIN Usage And Synthesis Chemical Properties:

dark brown crystalline powder HEMATEIN

Merck 13 Reference: Monograph Number: 0004651

Title: Hematein

CAS Registry Number: 475-25-2

CAS Name: 6a,7-Dihydro-3,4,6a,10-tetrahydroxybenz[b]indeno[1,2-d]pyran-9(6H)-one

Additional Names: hydroxybrasilein; hydroxybrazilein

Molecular Formula: C<sub>16</sub>H<sub>12</sub>O<sub>6</sub>

Molecular Weight: 300.26.

Percent Composition: C 64.00%, H 4.03%, O 31.97%

Literature References: Not to be confused with hematin. From hematoxylin or logwood extract and NH<sub>3</sub> by treatment with air: Engels et al., J. Chem. Soc. 93, 1115 (1908); Rolland, Teintex 3, 261, 322, 460 (1938); Justin-Mueller, Melliand Textilber. 30, 26, 63 (1949), C.A. 46, 8375h (1952).

Properties: Reddish-brown crystals with yellowish-green metallic luster. mp >200; also stated as 250 with decompn. Sol in about 1700 parts water; slightly sol in alcohol, ether; insol in benzene, chloroform; freely sol in ammonia with brownish-violet color and in dil NaOH with bright red color. Forms salts with heavy metals.

Melting point: mp >200; also stated as 250 with decompn

Use: As an indicator like hematoxylin; for staining animal tissue, particularly cell nuclei.