



Formula: C₃₀H₂₈O₈

MW: 516.55

CAS: 82-08-6

TNP NUMBER: TNP00157

MDL NUMBER: MFCD00017361

IUPAC: 3-[[8-((2E)-3-phenylprop-2-enoyl)-5,7-dihydroxy-2,2-dimethyl(2H-chromen-6-yl)]methyl]-1-acetyl-2,4,6-trihydroxy-5-methylbenzene

Smiles:

c1(c(Cc2c(c(c(c(c2O)C(=O)C)O)C)O)c(c2c(OC(C=C2)(C)C)c1C(=O)/C=Cc1cccc1)O)O

Principal phenolic component of kamala, q.v., an anthelmintic dye obtained from *Mallotus philippinensis* (Lam.) Muell. Arg, Euphorbiaceae.

REFERENCE: Gschwendt, M., et al. *Biochem. Biophys. Res. Commun.* 199, 93, (1994) abstract
 Haoyu Zeng, et al., , *Mallotoxin Is a Novel Human Ether-a-go-go-Related Gene (hERG) Potassium Channel Activator* *J. Pharmacol. Exp. Ther.* 319, 957-962, (2006) abstract
 Zakharov, S.I., et al., *Activation of the BK (SLO1) Potassium Channel by Mallotoxin* *J. Biol. Chem.* 35, 30882-30887, (2005) Gschwendt, M., et al. *FEBS Lett.* 338, 85, (1994)

SOURCE: Principal phenolic component of kamala, q.v., an anthelmintic dye obtained from *Mallotus philippinensis* (Lam.) Muell. Arg, Euphorbiaceae.

ACCEPTORS: 8

DONORS: 5

ROTATION BONDS: 10

N+O: 8

Chiral Centers: 0

LogP: 5.31

LogS: -5.67

LIPINSKI: 3

Monograph Number: 0008352

Title: Rottlerin

CAS Registry Number: 82-08-6

CAS Name:

(E)-1-[6-[(3-Acetyl-2,4,6-trihydroxy-5-methylphenyl)methyl]-5,7-dihydroxy-2,2-dimethyl-2H-1-benzopyran-8-yl]-3-phenyl-2-propen-1-one

Additional Names:

5,7-dihydroxy-2,2-dimethyl-6-(2,4,6-trihydroxy-3-methyl-5-acetylbenzyl)-8-cinnamoyl-1,2-chromene; mallotoxin

Molecular Formula: C₃₀H₂₈O₈

Molecular Weight: 516.54.

Percent Composition: C 69.76%, H 5.46%, O 24.78%

Literature References: Principal phenolic component of kamala, q.v., an anthelmintic dye obtained from *Mallotus philippinensis* (Lam.) Muell. Arg. (also known as *Rottlera tinctoria* Roxb.), Euphorbiaceae. Isoln: H. Telle, Arch. Pharm. 244, 446 (1906); S. Dutt, J. Chem. Soc. 127, 2044 (1925); A. McGookin et al., ibid. 1937, 748. Structure: Brockmann, Maier, Ann. 535, 149 (1938); A. McGookin et al., J. Chem. Soc. 1939, 1579. Synthesis of tetrahydrorottlerin: Backhouse et al., ibid. 1948, 113. Review of isoln and chemistry: M. Lounasmaa et al., Planta Med. 28, 16 (1975). Activity as protein kinase inhibitor: M. Gschwendt et al., Biochem. Biophys. Res. Commun. 199, 93 (1994). HPTLC determ in serum and pharmacokinetics: V. D. Mody et al., J. Pharm. Technol. 10, 71 (1994).

Properties: Light reddish-brown plates or needles with golden lustre from ethyl acetate, mp 212 (McGookin). Also reported as brownish-yellow plates from toluene, mp 206-207 (Dutt). Sol in ether, chloroform, benzene, ethyl acetate; sparingly sol in cold alc, acetic acid. Practically insol in water.

Melting point: mp 212 (McGookin); mp 206-207 (Dutt)

Derivative Type: 5,7-Dimethyl ether

Molecular Formula: C₃₂H₃₂O₈

Molecular Weight: 544.59.

Percent Composition: C 70.57%, H 5.92%, O 23.50%

Properties: Yellow crystals from ethyl acetate + acetone or chloroform + methanol, dec 245-246. Sol in chloroform, pyridine, hot glacial acetic acid; slightly sol in cold methanol, ethyl acetate, acetone, benzene, ether.

Derivative Type: Pentamethyl ether

Molecular Formula: C₃₅H₃₈O₈

Molecular Weight: 586.67.

Percent Composition: C 71.65%, H 6.53%, O 21.82%

Properties: Crystals from petr ether, methanol or 90% alcohol, mp 144. Very sol in acetone, glacial acetic acid, benzene, ethyl acetate.

Melting point: mp 144

Derivative Type: Pentaacetate

Molecular Formula: C₄₀H₃₈O₁₃

Molecular Weight: 726.72.

Percent Composition: C 66.11%, H 5.27%, O 28.62%

Properties: Leaflets from benzene + alcohol or acetone + alcohol, prisms from ethyl acetate, mp 212.

Melting point: mp 212

Derivative Type: Tetrahydrorottlerin

Molecular Formula: C₃₀H₃₂O₈

Molecular Weight: 520.57.

Percent Composition: C 69.22%, H 6.20%, O 24.59%

Properties: Yellow prisms from alcohol, mp 214.

Melting point: mp 214

Synonyms:

MALLOTOXIN;3'-[(8-CINNAMOYL-5,7-DIHYDROXY-2,2-DIMETHYL-2H-1-BENZOPYRAN-6-YL)METHYL]-2',4',6'-TRIHYDROXY-5'-METHYLACETOPHENONE;4