



Formula: C₃₀H₃₀O₈

MW: 518.56

CAS: 303-45-7

TNP NUMBER: TNP00355

MDL NUMBER: MFCD00017352

IUPAC: 7-[8-formyl-1,6,7-trihydroxy-3-methyl-5-(methylethyl)(2-naphthyl)]-2,3,8-trihydroxy-6-methyl-4-(methylethyl)naphthalenecarbaldehyde

Smiles: c1(c2c(c(c(c1O)O)C=O)c(c(c(c2)C)c1c(cc2c(c1O)c(c(c(c2C(C)C)O)O)C=O)C)O)C(C)C

M.P. 199 oC

http://chem.sis.nlm.nih.gov/chemidplus/ProxyServlet?objectHandle=DBMaint&actionHandle=default&nextPage=jsp/chemidheavy/ResultScreen.jsp&ROW_NUM=0&TXTSUPERLISTID=000303457

THERAPEUTIC CATEGORY: an antiviral at low concentration; antiherpes, antipsoriasis and antikeratitis, male contraceptive.

REFERENCE: Nadakavukaren MJ, Sorensen RH, Tone JN. Cell Tissue Res. 204:293-6 (1979). Sakesena SK, Salmonsens R, Lau IF, Chang MC. Contraception. 24:203-14 (1981). Tuszynski GP, Cossu G. Cancer Res. 44:768-71 (1984). Mego M. Bratisl Lek Listy. 103:378-81 (2002). 1. Lee et al., Mol. Cell. Biochem. (1982) 47:65 2. Abou-Donia et al., J. Agr. Food Chem. (1970). 18:534 3. Abou-Donia et al., Lipids (1970). 5(11):938 4. Bakhuni et al., Experienta 24:109 (1968). 24:109

SOURCE: From Cotton seeds.

ACCEPTORS: 8

DONORS: 6

ROTATION BONDS: 11

N+O: 8

Chiral Centers: 0

LogP: 7.27

LogS: -5.82

LIPINSKI: 1

Monograph Number: 0004543

Title: Gossypol

CAS Registry Number: 303-45-7

CAS Name: 1,1