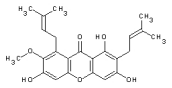

Formula: C24H26O6

MW: 410.47

CAS: 6147-11-1

MDL: MFCD00135200

TNP: TNP00140

1,3,6-Trihydroxy-7-methoxy-2,8-bis(3-methyl-2-butenyl)-9H-xanthen-9-one; 1,3,6-TRIHYDROXY-7-METHOXY-2,8-DI(3-METHYL-2-BUTENYL)XANTHONE; Mangosteen; mangostin; MANGOSTINE; Momordica Fruit P.E.; Fructus Monordicae extract; 1,3,6-Trihydroxy-7-methoxy-2,8-bis(3,3-di

LogP: 0.74

LogS: -3.05

Acceptors: 6

Donors: 3

Rotation Bonds: 8

Chiral Centers: 0

N+O: 6

LIPINSKY: 4

IUPAC: 1,7-bis(3-methylbut-2-enyl)-3,6,8-trihydroxy-2-methoxyxanthen-9-one

Smiles: c12c(c3c(c(c(O)cc3oc2cc(c(c1O)CC=C(/C)C)O)OC)CC=C(C)C)=O

SOURCE: From various parts of mangosteen tree

Specification: Xanthones; Intermediates & Fine Chemicals; Pharmaceuticals Mangostin Chemical Properties:

 mp 180-182C CAS DataBase Reference6147-11-1(CAS DataBase Reference) Mangostin Usage And Synthesis Chemical Properties:

Yellow Crystalline Solid UsageIt was isolated from Garcinia mangostana Linn (Guttiferae). It is an anti-inflammatory agent Mangostin

Merck 13 Reference: Monograph Number: 0005766

Title: Mangostin

CAS Registry Number: 6147-11-1

CAS Name: 1,3,6-Trihydroxy-7-methoxy-2,8-bis-(3-methyl-2-butenyl)-9H-xanthen-9-one

Additional Names: 1,3,6-trihydroxy-7-methoxy-2,8-di(3-methyl-2-butenyl)xanthone

Molecular Formula: C24H26O6

Molecular Weight: 410.46.

Percent Composition: C 70.23%, H 6.38%, O 23.39%

Literature References: From various parts of the mangosteen tree (Garcinia mangostana L., Guttiferae): Schmid, Ann. 93, 83 (1855); Dragendorff, ibid. 482, 280 (1930). Structure: Yates, Stout, J. Am. Chem. Soc. 80, 1691 (1958); Scheinmann, Chem. Commun. 1967, 1015; Stout et al., ibid. 1968, 211.

Properties: Yellow crystals from benzene, mp 181.6-182.6. uv max (ethanol): 243, 259, 318, 351 nm (log e 4.54, 4.44, 4.38, 3.86). Practically insol in water; sol in alcohol, ether, acetone, chloroform, ethyl acetate.

Melting point: mp 181.6-182.6

Absorption maximum: uv max (ethanol): 243, 259, 318, 351 nm (log e 4.54, 4.44, 4.38, 3.86)

Derivative Type: 3,6-Dimethylmangostin

Molecular Formula: C26H30O6

Molecular Weight: 438.51.

Percent Composition: C 71.21%, H 6.90%, O 21.89%

Properties: Pale yellow needles from ethanol, mp 123.3-123.8. uv max (ethanol): 245, 262, 314, 350 nm (log e 4.50, 4.53, 4.36, 3.81).

Melting point: mp 123.3-123.8

Absorption maximum: uv max (ethanol): 245, 262, 314, 350 nm (log e 4.50, 4.53, 4.36, 3.81)