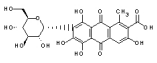

Formula: C22H20O13

MW: 492.39

CAS: 1260-17-9

MDL: MFCD00062965

TNP: TNP00410

cochenilledye; cochineal(dye); FD AND C CARMINE; E120; CALCIUM ALUMINIUM LACQUER WITH CARMINIC ACID; CARMINATE BORAX; CARMINE 2G; CARMINE 40

LogP: 5.66

LogS: -5.27

Acceptors: 13

Donors: 9

Rotation Bonds: 7

Chiral Centers: 5

N+O: 13

LIPINSKY: 2

IUPAC: 7-[(5S,2R,3R,4R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropy ran-2-yl)]-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxoanthracene-2-carboxylic aci d

Smiles: c1([C@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O)O)O)c(c(O)c2c(c1O)C(c1c(cc(c(c1C)C(=O)O)O)C2=O)=O)O

SOURCE: Glucosidal coloring matter from the scale insect Coccus Cati L., Homoptera

Specification: Anthraquinones; Hydroxyanthraquinones CARMINE Chemical Properties:

Colour Index 75470 Merck 2457 Safety 22-24/25 WGK Germany 2 RTECS GG5350000 CARMINE Usage And Synthesis CARMINE Preparation ProductsKARAYA GUM-->CARMINE Raw materialsCARMINE

Merck 13 Reference: Monograph Number: 0001855

Title: Carminic Acid

CAS Registry Number: 1260-17-9

CAS Name:
7-a-D-Glucopyranosyl-9,10-dihydro-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid

Additional Names: C.I. Natural Red 4; C.I. 75470

Molecular Formula: C22H20O13

Molecular Weight: 492.39.

Percent Composition: C 53.66%, H 4.09%, O 42.24%

Literature References: Glucosidal coloring matter from the scale insect Coccus cacti L., Homoptera (cochineal). The essential constituent of carmine. Isoln: Schunk, Marchlewski, Ber. 27, 2979 (1894); Dimroth, Scheuer, Ann. 399, 43 (1913). Structure: Dimroth, Kammerer, Ber. 53, 471 (1920); Ali, Haynes, J. Chem. Soc. 1959, 1033; revised structure: Bhatia, Venkataraman, Indian J. Chem. 3 (2), 92 (1965). See also Colour Index vol. 4 (3rd ed., 1971) p 4632.

Properties: Red prisms from alc, no distinct melting point, darkens at 120. Has a deep red color in water and is yellow to violet in acid solns. uv max (water): 500 nm (e 6800); (0.02N HCl): 490-500 nm (e 5800); (0.0001N NaOH): 540 nm (e 3450). [a]15654 +51.6 (water). Sol in water, alc, concd H2SO4; slightly sol in ether. Practically insol in petr ether, benzene, chloroform.

Optical Rotation: [a]15654 +51.6 (water)

Absorption maximum: uv max (water): 500 nm (e 6800); (0.02N HCl): 490-500 nm (e 5800); (0.0001N NaOH): 540 nm (e 3450)

Derivative Type: Methyl tetra-O-methylcarminate

Molecular Formula: C27H30O13

Molecular Weight: 562.52.

Percent Composition: C 57.65%, H 5.38%, O 36.98%

Properties: Yellow needles from benzene + petr ether, mp 185-188.

Melting point: mp 185-188

Derivative Type: Aluminum calcium lake

Additional Names: Carmine

Properties: Bright-red, light pieces; easily reduced to powder. Practically insol in cold water or dil acids. Partly sol in hot water; sol in solns of alkali hydroxides or their carbonates giving deep red solns; also sol in borax.

Use: Free acid in color photography; pigment for artists' paints; as bacteriol. stain; rarely now as acid-base indicator or as oxidimetric indicator; as a reagent for aluminum; as a complexing agent for cations. Aluminum calcium lake as dye; in inks; coloring foods, drugs and galenicals; in microscopy for making various stains.