



Formula: C₁₄H₈O₅

MW: 256.21

CAS: 81-54-9

MDL: MFCD00001203

TNP: TNP00463



LogP: 2.39

LogS: -3.65

Acceptors: 5

Donors: 3

Rotation Bonds: 3

Chiral Centers: 0

N+O: 5

LIPINSKY: 4

Info: Purpurin, occurs as glycoside in madder root. It is formed during storage

IUPAC: 1,2,4-trihydroxyanthracene-9,10-dione

Smiles: c12c(C(=O)c3c(C1=O)cccc3)c(O)c(cc2O)O

Merck 13 Reference: Monograph Number: 0008036

Title: Purpurin

CAS Registry Number: 81-54-9

CAS Name: 1,2,4-Trihydroxy-9,10-anthracenedione

Additional Names: 1,2,4-trihydroxyanthraquinone; C.I. Natural Red 8; C.I. Natural Red 16; C.I. 58205; C.I. 75410

Molecular Formula: C₁₄H₈O₅

Molecular Weight: 256.21.

Percent Composition: C 65.63%, H 3.15%, O 31.22%

Literature References: Occurs as glycoside in the madder root (*Rubia tinctorum* L., Rubiaceae) of commerce. Is formed during storage; no appreciable amount in the fresh root: Hill, Richter, J. Chem. Soc. 1936, 1714. Although a dye itself, it is usually considered as an undesirable contaminant of alizarin extracted from madder. May be prepd from alizarin by oxidation with ammonium persulfate: Wacker, J. Prakt. Chem. [2] 54, 90 (1896); also by Friedel-Crafts condensation of hydroxyhydroquinone with phthalic anhydride: Dimroth, Fick, Ann. 411, 321 (1916).

Properties: Long orange needles with 1 H₂O from dil alcohol, anhydr at 100. Anhydr red needles from abs alcohol or by sublimation around 150 in high vacuum (less than 2 mm Hg). mp 257. Absorption spectrum: Meek, J. Chem. Soc. 111, 969 (1917); Ezaby, ibid. (B) 1970, 1293. More sol in boiling water than alizarin (yellow color with yellowish hue). Freely sol in alcohol (red), in ether (intensely yellow with fluorescence). Soluble in benzene, toluene, xylene (dark yellow), in boiling alum soln (red).

Melting point: mp 257

Derivative Type: 2-Methyl ether

Molecular Formula: C₁₅H₁₀O₅

Molecular Weight: 270.24.

Percent Composition: C 66.67%, H 3.73%, O 29.60%

Properties: Orange crystals from benzene, mp 240.

Melting point: mp 240

Derivative Type: 2,4-Dimethyl ether

Molecular Formula: C₁₆H₁₂O₅

Molecular Weight: 284.26.

Percent Composition: C 67.60%, H 4.26%, O 28.14%

Properties: Orange needles, mp 186-189.

Melting point: mp 186-189

Use: Forms colored