



Formula: C₁₅H₁₀O₄

MW: 254.24

CAS: 481-74-3

MDL: MFCD00001208

TNP: TNP00557

CHRY SOPHANIC ACID; CHRY SOPHANOL; 3-METHYLCHRYSAZIN;
3-METHYLCHRYSAZINE; 9,10-ANTHRACENEDIONE, 1,8-DIHYDROXY-3-METHYL;
1,8-DIHYDROXY-3-METHYL-9,10-ANTHRACENEDIONE;
1,8-DIHYDROXY-3-METHYLANTHRAQUINONE; RHUBARB EXTRACT



LogP: 1.47

LogS: -3.35

Acceptors: 4

Donors: 2

Rotation Bonds: 2

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

Info: Chrysophanic acid 98%

IUPAC: 1,8-dihydroxy-3-methylanthracene-9,10-dione

Smiles: c12C(c3c(O)cccc3C(c1cc(cc2O)C)=O)=O

SOURCE: Occurs in cascara sagrada, senna and various species of Rumex and Rheum

Specification: Anthraquinones, Hydroquinones and Quinones; The group of Polydatin
Chrysophanic acid Chemical Properties:

mp 194-198 C Water Solubility