



Formula: C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>

MW: 270.24

CAS: 518-82-1

TNP NUMBER: TNP00318

MDL NUMBER: MFCD00001207

IUPAC: 1,6,8-trihydroxy-3-methylanthracene-9,10-dione

Smiles: C1(c2c(C(=O)c3c1c(cc(C)c3)O)cc(cc2O)O)=O

SOURCE: from Frangula bark, >90% (HPLC), powder

ACCEPTORS: 5

DONORS: 3

ROTATION BONDS: 3

N+O: 5

Chiral Centers: 0

LogP: 0.87

LogS: -3.07

LIPINSKI: 4

Synonyms:

1,3,8-trihydroxy-6-methyl-10-anthracenedione;1,3,8-trihydroxy-6-methyl-anthraquinon;6-methyl-1,3,8-trihydroxy-anthraquinon;persianberrylake;schuttgelb;RHUBARB EXTRACT;RHEUM EMODIN;FRANGULA EMODIN

CAS:518-82-1

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MW:270.24

EINECS:208-258-8

Product Categories:Anthraquinones, Hydroquinones and Quinones;Anthraquinones;Hydroxyanthraquinones;Natural Plant Extract;The group of Polydatin;Protein Kinase;plant extract;Nutritional Ingredients;reference substance Emodin

Chemical Properties: mp 255 C (dec.)(lit.) storage temp. 2-8C solubility DMSO: soluble form powder color orange Water Solubility