



Formula: C₁₁H₈O₃

MW: 188.18

CAS: 481-42-5

MDL: MFCD00001682

TNP: TNP00543

5-HYDROXY-2-METHYL-1,4-NAPHTHOQUINONE;
5-HYDROXY-2-METHYL-1,4-NAPHTHOQUINONE; PLUMBAGAN; PLUMBAGIN; SPECS
AP-782/41885488; RARECHEM BW GA 0426; 2-methyl-5-hydroxy-1,4-naphthoquinone;
2-methyljuglone



LogP: 0.43

LogS: -4.36

Acceptors: 3

Donors: 1

Rotation Bonds: 1

Chiral Centers: 0

N+O: 3

LIPINSKY: 4

IUPAC: 5-hydroxy-2-methylnaphthalene-1,4-dione

Smiles: c1cc(c2C(C=C(C(c2c1)=O)C)=O)O

Specification: Anthraquinones, Hydroquinones and Quinones PLUMBAGIN Chemical

Properties:

mp 76-78 C(lit.) storage temp. -20C Merck 7538 Safety Information Hazard Codes T Risk Statements 25-34 Safety Statements 22-26-36/37/39-45 RIDADR UN 2923 8/PG 2 WGK Germany 3 RTECS QL8500000 Hazard Note Toxic HazardClass 6.1(a) PackingGroup I I PLUMBAGIN Usage And Synthesis Chemical Properties:

ORANGE CRYSTALLINE POWDER OR CRYSTALS PLUMBAGIN Raw materials Ethyl acetate-->Dichloromethane-->Acetic acid glacial-->Magnesium sulfate-->Sodium bicarbonate-->Aluminium chloride-->1,4-Dioxane-->Iodomethane-->Magnesium-->Acetyl chloride-->N-Bromosuccinimide-->Sulfuryl chloride-->Nitrobenzene-->Cuprous bromide-->Tin tetrachloride-->Tetrakis(triphenylphosphine)palladium-->1,4-Diamino anthraquinone-->1,4-Diamino-2,3-dihydroanthraquinone-->1,5-Dihydroxy naphthalene

Merck 13 Reference: Monograph Number: 0007621

Title: Plumbagin

CAS Registry Number: 481-42-5

CAS Name: 5-Hydroxy-2-methyl-1,4-naphthalenedione

Additional Names: 5-hydroxy-2-methyl-1,4-naphthoquinone

Molecular Formula: C₁₁H₈O₃

Molecular Weight: 188.18.

Percent Composition: C 70.21%, H 4.29%, O 25.51%

Literature References: Found in the roots of *Plumbago europaea* L., *P. zeylanica*, *P. rosea* L., Plumbaginaceae. Isoln: Dulong d'Astafort, *J. Pharm. Chim.* 14, 441 (1828); Wefers-Bettink, *Rec. Trav. Chim.* 8, 319 (1889); Ray, Dutt, *J. Indian Chem. Soc.* 5, 419 (1928). Structure and synthesis: Fieser, Dunn, *J. Am. Chem. Soc.* 58, 572 (1936). Biosynthesis: Durand, Zenk, *Tetrahedron Lett.* 1971, 3009. Chemotherapeutic properties: Vichkanova et al., *C.A.* 78, 66906s (1973). Efficient syntheses: A. Ichihara et al., *Agric. Biol. Chem.* 44, 211 (1980); G. Wurm et al., *Arch. Pharm.* 314, 861, 1055 (1981); H. M