



Formula: C₁₁H₈O₂

MW: 172.18

CAS: 58-27-5

MDL NUMBER: MFCD00001681

IUPAC: 2-methylnaphthalene-1,4-dione

Smiles: C1(C(=CC(=O)c2c1cccc2)C)=O

THERAPEUTIC CATEGORY: Vitamin (Prothrombogenic)

ACCEPTORS: 2

DONORS: 0

ROTATION BONDS: 0

N+O: 2

Chiral Centers: 0

LogP: 1.25

LogS: -3.15

LIPINSKI: 4

Synonyms:

2-METHYLNAPHTHOQUINONE;2-METHYL-1,4-DIHYDRONAPHTHALENE-1,4-DIONE;2-METHYL-1,4-NAPHTHOQUINONE;2-METHYL-1,4-NAPHTHAQUINONE;MENAPHTHON;MENAPHTHONONE;MENADIONE;THYLOQUINONE

CAS:58-27-5

MF:C11H8O2

MW:172.18

EINECS:200-372-6

Product Categories:Biochemistry;Vitamins;Nutritional fortification substances;Vitamins and derivatives;Vitamin Ingredients;Miscellaneous Compounds Menadione

Chemical Properties: mp 105-107 C(lit.) storage temp. Store at RT. solubility oil: soluble form crystalline color yellow Water Solubility INSOLUBLE Sensitive Light Sensitive Merck 14,5831 BRN 1908453 Stability:Stable. May be light sensitive. Incompatible with strong oxidizing agents.

CAS DataBase Reference: 58-27-5(

CAS DataBase Reference:) NIST Chemistry ReferenceMenadione(58-27-5) EPA Substance Registry System1,4-Naphthalenedione, 2-methyl-(58-27-5) Xn,Xi Risk Statements 22-36/37/38-43 Safety Statements 26-36-37/39-24 WGK Germany 3 RTECS QL9100000 F 8 Hazardous Substances Data58-27-5(Hazardous Substances Data) Menadione

Usage And Synthesis:

Chemical Properties: Bright yellow crystals Menadione

