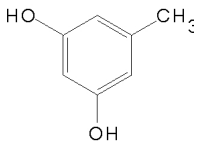

Formula: C7H8O2

MW: 124.14

Salt: H2O

CAS: 504-15-4

MDL: MFCD00002291

TNP: TNP00515

ORCINOL; TIMTEC-BB SBB006928; 3,5-DIHYDROXYTOLUENE; AKOS 92132; 5-METHYLRESORCINOL; 5-METHYL-1,3-BENZENEDIOL; 2,6-DIMETHYLRESORCINOL; 1,3-DIHYDROXY-5-METHYLBENZENE

LogP: 1.49

LogS: -3.44

Acceptors: 2

Donors: 2

Rotation Bonds: 2

Chiral Centers: 0

N+O: 2

LIPINSKY: 4

Info: Occurs in many species of lichens

IUPAC: 5-methylbenzene-1,3-diol

Smiles: c1c(cc(C)cc1O)O

Specification: Alcohols and Derivatives; Aromatic Phenols Orcinol Chemical Properties:

 mp 106-112 C(lit.) bp 290 C Fp 159 C Sensitive Air Sensitive Merck 14,6864 BRN 1071903 CAS DataBase Reference504-15-4(CAS DataBase Reference) NIST Chemistry Reference3,5-Dihydroxytoluene(504-15-4) EPA Substance Registry System1,3-Benzenediol, 5-methyl-(504-15-4) Safety Information Hazard Codes Xn Risk Statements 22-36/37/38-41-37/38-20/21/22 Safety Statements 22-26-36-37/39 RIDADR 2811 WGK Germany 3 RTECS VH2100000 PackingGroup III HS Code 29072900 1,3-Dihydroxy-5-methylbenzene English Orcinol Usage And Synthesis Chemical Properties:

pink-grey to pink-brown cryst. powder or crystals Orcinol

Merck 13 Reference: Monograph Number: 0006932

Title: Orcinol

CAS Registry Number: 504-15-4

CAS Name: 5-Methyl-1,3-benzenediol

Additional Names: 5-methylresorcinol; orcin; 3,5-dihydroxytoluene

Molecular Formula: C7H8O2

Molecular Weight: 124.14.

Percent Composition: C 67.73%, H 6.50%, O 25.78%

Literature References: Occurs in many species of lichens: Sastry, Rao, Curr. Sci. 10, 437 (1941). Prepn: Anker, Cook, J. Chem. Soc. 1945, 311; Kisteneva, Rozhdestvenskii, Zh. Prikl. Khim. 22, 1108 (1949); Stevens, US 2603662 (1952 to Gulf); Zimmer, US 3028410 (1962 to Hooker Chem.). Toxicity studies: I. Veldre et al., Vopr. Gig. Tr. Prof. Patol. Est. SSR 2, 160 (1970), C.A. 74, 51746h (1971).

Derivative Type: Monohydrate

Properties: Crystals; sweet but unpleasant taste; reddens on exposure to air due to oxidation. mp about 58; 107 when anhydr. bp 290; bp14-20 165-170; bp5 147. Freely sol in water, alcohol, ether; less sol in benzene; slightly sol in chloroform or carbon disulfide. Keep well closed and protected from light. LD50 in mice, rats, rabbits, guinea pigs (mg/kg): 772, 844, 2400, 1678 orally (Veldre).

Melting point: mp about 58; 107 when anhydr

Boiling point: bp 290; bp14-20 165-170; bp5 147

Toxicity data: LD50 in mice, rats, rabbits, guinea pigs (mg/kg): 772, 844, 2400, 1678 orally (Veldre)

Use: As a reagent for pentoses, lignin, beet sugar, saccharoses, arabinose, diastase.