



Formula: C<sub>21</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>

MW: 362.39

Salt: Mixture of several compounds.

CAS: 1400-62-0

MDL: MFCD00064592

TNP: TNP00347

NATURAL RED 28; ORCEIN; ORCEIN, NATURAL; ORCEIN STAINING; ORCEIN SYNTHETIC; Orceinforanalysis; ORCEIN, SYNTHETIC, CERTIFIED; Trifloxysulfuron Sodium Salt, Pestanal



LogP: 3.45

LogS: -4.73

Acceptors: 4

Donors: 4

Rotation Bonds: 3

Chiral Centers: 0

N+O: 6

LIPINSKY: 4

IUPAC: 7-amino-8-(2,4-dihydroxy-6-methylphenyl)-1,9-dimethylphenoxazin-3-one

Smiles: Cc1c(c2c(c3nc4c(cc(cc4C)=O)oc3cc2N)C)c(cc(c1)O)O

Specification: ORCEIN Chemical Properties:

storage temp. Store at RT. Merck 14,6863 Stability:Stable. Safety Information Hazard Codes Xn Risk Statements 22 Safety Statements 37/39-26 WGK Germany 3 ORCEIN Usage And Synthesis Chemical Properties:

dark brown crystals or powder ORCEIN

Merck 13 Reference: Monograph Number: 0006931

Title: Orcein

CAS Registry Number: 1400-62-0

Literature References: A dye first prepared from lichens (cudbear, q.v., or archil). Prepn by oxidation of orcinol with H<sub>2</sub>O<sub>2</sub> in the presence of ammonia water: Zulkowski, Peters, Monatsh. Chem. 11, 227 (1890). Can be separated into 14 dyes by distribution chromatography: Musso, Ber. 89, 1659 (1956). The eight compds depicted are the major components of orcein; b- and g-components are cis-trans isomers of the same compd. Structure studies: Beecken et al., Angew. Chem. 73, 665 (1961). Brief review: H. J. Conn's Biological Stains, R. D. Lillie, Ed. (Williams & Wilkins, Baltimore, 9th ed., 1977) pp 400-403. Review of use as textile dye and histological stain for elastin: H. Puchter, S. N. Meloan, Histochemistry 64, 119 (1979).

Properties: Brownish-red microcryst powder. Practically insol in water, benzene, chloroform, ether, carbon disulfide. Sol in alcohol, acetone or acetic acid with red color, in dil aq alkali with bluish-violet color.

Use: Biological stain.