



Formula: C₆H₆O₄

MW: 142.11

CAS: 501-30-4

TNP NUMBER: TNP00261

MDL NUMBER: MFCD00006580

IUPAC: 5-hydroxy-2-(hydroxymethyl)pyran-4-one

Smiles: c1(c(cc(oc1)CO)=O)O

ACCEPTORS: 4

DONORS: 2

ROTATION BONDS: 3

N+O: 4

Chiral Centers: 0

LogP: -1.65

LogS: -1.88

LIPINSKI: 4

Monograph Number: 0005334

Title: Kojic Acid

CAS Registry Number: 501-30-4

CAS Name: 5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one

Additional Names: 5-hydroxy-2-(hydroxymethyl)-4-pyrone;
2-hydroxymethyl-5-hydroxy-g-pyrone

Molecular Formula: C₆H₆O₄

Molecular Weight: 142.11.

Percent Composition: C 50.71%, H 4.26%, O 45.03%

Literature References: Antibiotic substance produced in an aerobic process by a variety of microorganisms from a wide range of carbon sources. Isolation from *Aspergillus oryzae*: Saito, Bot. Mag. Tokyo 21, 249 (1907). Structure: Yabuta, J. Chem. Soc. 125, 575 (1924); Heyns, Vogelsang, Ber. 87, 13 (1954). Synthesis: Stacey, Turton, J. Chem. Soc. 1946, 661; Lichtenthaler, Heidel, Angew. Chem. Int. Ed. 8, 978 (1968). Industrial prep: GB 826244 (1959 to Pfizer), C.A. 54, 11372e (1960). Mutagenicity study: C. I. Wei et al., Toxicol. Lett. 59, 213 (1991). Review: Be