



Formula: C₉H₆O₂

MW: 146.15

CAS: 91-64-5

MDL: MFCD00006850

TNP: TNP00433

TIMTEC-BB SBB000094; O-HYDROXYCINNAMIC ACID LACTONE; TONKA BEAN CAMPHOR; 5,6-BENZO-2-PYRONE; AKOS 212-75; 2H-1-BENZOPYRAN-2-ONE; 2H-1-BENZOPYAN-2-ONE; 1,2-BENZOPYRONE



LogP: -0.85

LogS: -2.09

Acceptors: 2

Donors: 0

Rotation Bonds: 0

Chiral Centers: 0

N+O: 2

LIPINSKY: 4

IUPAC: chromen-2-one

Smiles: o1c(ccc2c1cccc2)=O

SOURCE: In Tonka Beans, Lavander Oil, woodruff, sweet clover

Specification: FINE Chemical & INTERMEDIATES; Food & Feed ADDITIVES; Coumarins; Coumarin; Natural Plant Extract Coumarin Chemical Properties:

mp 68-73 C(lit.) bp 298 C(lit.) density 0.935 vapor pressure 0.01 mm Hg (47 C) Fp 162 C
Water Solubility 1.7 g/L (20