



Formula: C₁₈H₁₆O₇

MW: 344.32

CAS: 125-46-2

MDL: MFCD01457247

TNP: TNP00002

TIMTEC-BB SBB006458; (+)-USNEIN; (+)-USNIACIN; (r)-usnicaci;
3(2h,9bh)-dibenzofurandione,2,6-diacetyl-7,9-dihydroxy-8,9b-dimethyl-(9b);
6-diacetyl-1,7,9-trihydroxy-8,9b-dimethyl-d-3(9bh)-dibenzofuranon;
6-diacetyl-8,9b-dimethyl-1,7,9-trihydroxy-d-3(9bh)-dibenzof



LogP: 2.75

LogS: -3.8

Acceptors: 7

Donors: 2

Rotation Bonds: 4

Chiral Centers: 2

N+O: 7

LIPINSKY: 4

IUPAC: (9aR)-4,8-diacetyl-1,3-dihydroxy-2,9a-dimethyl-7,9-dioxo-8,9a-dihydrobenzo[2,1-d]benzo[b]furan

Smiles: C[C@@]12c3c(OC1=CC(C(C2=O)C(C)=O)=O)c(C(C)=O)c(c(c3O)C)O

SOURCE: (+)-Usnic acid from *Usnea dasypoga*,
2,6-Diacetyl-7,9-dihydroxy-8,9b-dimethyldibenzofuran-1,3(2H,9bH)-dione

Specification: Pharmaceutical Raw Materials; Plant Oils, Toxins, Phenolic Acids & Derivatives
(+)-Usniacin Chemical Properties:

mp 201-203 C(lit.) alpha 488