Formula: C6H6O3

MW: 126.11

CAS: 37112-31-5

TNP NUMBER: TNP00415

MDL NUMBER: MFCD00191664

IUPAC: 7,8-dioxabicyclo[3.2.1]oct-3-en-2-one

Smiles: C1OC2OC1C=CC2=O

Oil

Product of pyrolysis of cellulose.

ACCEPTORS: 3

DONORS: 0

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 2

LogP: -1.2

LogS: -2.12

LIPINSKI: 4

Synonyms:

(1s)-8-dioxabicyclo(3.2.1)oct-2-en-4-one;1,6-ANHYDRO-3,4-DIDEOXY-ALPHA-D-GLYCERO-H EX-3-ENOPYRANOSE-2-ULOSE;6,8-DIOXA-BICYCLO[3.2.1]OCT-2-EN-4-ONE;LEVOGLUCO SENONE;1,6-Anhydro-3,4-dideoxy-a-D-glycero-hex-3-enopyranose-2-ulose;6,8-Dioxabicyclo3. 2.1oct-2-en-4-one, (1S,5R)-;1,6-Anhydro-3,4-dideoxy-a-D-glycero-hex-3-enopyranose-2-ulose;(1S,5R)-6,8-Dioxabi cyclo[3.2.1]oct-2-en-4-one

CAS:37112-31-5

MF:C6H6O3

MW:126.11

EINECS:

Product Categories:Chiral Reagents;Heterocycles LEVOGLUCOSENONE LEVOGLUCOSENONE

Usage And Synthesis:

Chemical Properties: Colourless to Yellow Oil Usage(-)-Form is a pyrolysis product of cellulose and cellulose-containing materials including pulp and paper waste products. Known as a pyrolytic product of cellulose, its very useful as a chiral source for synthesizing natural products because of its LEVOGLUCOSENONE

MOLFILE