



Formula: C₆H₁₀O₄

MW: 146.14

CAS: 652-67-5

TNP NUMBER: TNP00593

MDL NUMBER: MFCD00014554

IUPAC: (2S,6R)-4,8-dioxabicyclo[3.3.0]octane-2,6-diol

Smiles: O1C2C(OC[C@@H]2O)[C@@H](O)C1

THERAPEUTIC CATEGORY: Diuretic

ACCEPTORS: 4

DONORS: 2

ROTATION BONDS: 0

N+O: 4

Chiral Centers: 4

LogP: -2.36

LogS: -1.71

LIPINSKI: 4

Synonyms:

1,4:3,6-DIANHYDRO-D-SORBITOL;1,4:3,6-DIANHYDROGLUCITOL;1,4:3,6-DIANHYDROSORBITOL;1,4:3,6-DIANHYDRO-D-GLUCITOL;(3S,3AR,6R,6AR)-HEXAHYDRO-FURO[3,2-B]FURAN-3,6-DIOL;D-ISOSORBIDE;DIANHYDRO-D-GLUCITOL;DIANHYDRO-D-SORBITOL

CAS:652-67-5

MF:C6H10O4

MW:146.14

EINECS:211-492-3

Product Categories: Isosorbide

Chemical Properties: mp 60-63 C(lit.) alpha 42 (c=3, H2O) refractive index 45 (C=5, H2O)
Sensitive Hygroscopic Merck 14,5224 BRN 80510

CAS DataBase Reference: 652-67-5(

CAS DataBase Reference:)

Safety Information: Risk Statements 22 Safety Statements 24/25 WGK Germany 2 RTECS
LZ4380000 Hazardous Substances Data652-67-5(Hazardous Substances Data) Isosorbide

Usage And Synthesis:

Chemical Properties: off-white to light yellow or beige crystals, Isosorbide

