



Formula: C7H12O6

MW: 192.17

CAS: 77-95-2

MDL: MFCD00065351

TNP: TNP00370

1,3,4,5-tetrahydroxy-, [1R-(1-.alpha.,3-.alpha.,4-.alpha.,5-.beta.)]-Cyclohexanecarboxylic acid;
3,4,5-tetrahydroxy-(-)-cyclohexanecarboxylic acid; 5-beta)-h; 5beta)]-alph; Chinasäure;
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, (-)-; cyclohexanecarboxylic acid



LogP: 1.86

LogS: -3.2

Acceptors: 6

Donors: 5

Rotation Bonds: 2

Chiral Centers: 2

N+O: 6

LIPINSKY: 4

IUPAC: (3R,5R)-1,3,4,5-tetrahydroxycyclohexanecarboxylic acid

Smiles: C1(CC(O)C(C(C1)O)O)(C(=O)O)O

Specification: chiral; for Resolution of Bases; Optical Resolution; Synthetic Organic Chemistry;
Asymmetric Synthesis; Chiral Resolution Reagents; Chiral Resolving Reagents Quinic acid

Chemical Properties:

mp 165-170 C alpha -44