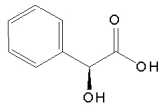

Formula: C8H8O3

MW: 152.15

CAS: 17199-29-0

MDL NUMBER: MFCD00004495

IUPAC: (2S)-2-hydroxy-2-phenylacetic acid

Smiles: C([C@H](c1ccccc1)O)(=O)O

THERAPEUTIC CATEGORY: ANTISEPTIC (URINARY)

ACCEPTORS: 3

DONORS: 2

ROTATION BONDS: 2

N+O: 3

Chiral Centers: 1

LogP: 0.83

LogS: -2.64

LIPINSKI: 4

Synonyms:
(s)-(+)-mandelic;(s)-benzeneaceticaci;(S)-Hydroxyphenylaceticacid;Benzeneaceticacid,alpha-hydroxy-,(S)-;L-mandelate;L-ALPHA-HYDROXYPHENYLACETIC ACID;L-A-HYDROXYPHENYLACETIC ACID;L-AMYGDALIC ACID

CAS:17199-29-0

MF:C8H8O3

MW:152.15

EINECS:241-240-8

Product Categories:FINE Chemical & INTERMEDIATES;Chiral Compounds;Aromatic Phenylacetic Acids and Derivatives;chiral;Analytical Chemistry;Carboxylic Acids (Chiral);Chiral Building Blocks;e.e. / Absolute Configuration Determination (NMR);Enantiomer Excess & Absolute Configuration Determination;for Resolution of Bases;Optical Resolution;Synthetic Organic Chemistry;Chiral Compound (S)-(+)-Mandelic acid

Chemical Properties: mp 131-134 C(lit.) alpha 155 (c=2 , H2O) refractive index 153.5 (C=1, H2O) Water Solubility 100 g/L (25 C) Sensitive Light Sensitive BRN 2208678 Stability:Stable, but light sensitive. Combustible. Incompatible with strong bases, strong oxidizing agents, strong reducing agents.

CAS DataBase Reference: 17199-29-0(

CAS DataBase Reference:) NIST Chemistry ReferenceBenzeneacetic acid,