



>>Entry Name: 3-Hydroxypentanedioic acid, 9CI

Synonym(s): 3-Hydroxyglutaric acid, 8CI. 2-Hydroxypropane-1,3-dicarboxylic acid

CAS Registry Number: 638-18-6

HOOCCH<sub>2</sub>CH(OH)CH<sub>2</sub>COOH

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>5</sub>

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Physical Description: Needles (H<sub>2</sub>O)

Melting Point: Mp 95°

Solubility: Sol. H<sub>2</sub>O, EtOH, spar. sol. Et<sub>2</sub>O

>>Derivative: Di-Me ester

CAS Registry Number: 7250-55-7

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O<sub>5</sub>

Molecular Weight: 176.169

Accurate Mass: 176.068475

Percentage Composition: C 47.73%; H 6.87%; O 45.41%

Boiling Point: Bp<sub>10</sub> 134-136°

Aldrich: 16697-9

Fluka: 55275

Rare Chemicals Library: S36103-8

>>Derivative: Di-Et ester

CAS Registry Number: 32328-03-3

Molecular Formula: C<sub>9</sub>H<sub>16</sub>O<sub>5</sub>

Molecular Weight: 204.222

Accurate Mass: 204.099775

Percentage Composition: C 52.93%; H 7.90%; O 39.17%

Boiling Point: Bp<sub>2</sub> 105-107°

Aldrich: D9700-2

Fluka: 55270

>>Derivative: Ac

Molecular Formula: C<sub>7</sub>H<sub>10</sub>O<sub>6</sub>

Molecular Weight: 190.152

Accurate Mass: 190.04774

Percentage Composition: C 44.22%; H 5.30%; O 50.48%

Melting Point: Mp 65-66°

pKa Value: pK<sub>a</sub> 3.8

>>Derivative: Dinitrile

Synonym(s): 1,3-Dicyano-2-propanol

CAS Registry Number: 13880-89-2

Molecular Formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

Physical Description: Yellow oil

Boiling Point: Bp<sub>0.2</sub> 154-156°

Density: d<sub>4</sub><sup>35</sup> 1.01

>>Derivative: Dinitrile, Ac

Synonym(s): 2-Acetoxy-1,3-dicyanopropane

Molecular Formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Physical Description: Liq.

Melting Point: Mp 45°

Boiling Point: Bp<sub>1</sub> 126.5°