



**>>Entry Name: 3,3'-Iminobispropanoic acid**

**Synonym(s):** *N*-(2-Carboxyethyl)-β-alanine, 9CI. 3,3'-Iminodipropionic acid. 3,3'-Iminobispropionic acid. Diethylamine-β,β'-dicarboxylic acid. 4-Azapimelic acid

**CAS Registry Number:** 505-47-5

HOOCCH<sub>2</sub>CH<sub>2</sub>NHCH<sub>2</sub>CH<sub>2</sub>COOH

**Molecular Formula:** C<sub>6</sub>H<sub>11</sub>NO<sub>4</sub>

**Molecular Weight:** 161.157

**Accurate Mass:** 161.068809

**Percentage Composition:** C 44.72%; H 6.88%; N 8.69%; O 39.71%

**Melting Point:** Mp 151-151.5°

**pKa Value:** p*K*<sub>a</sub> 4.2

**>>Derivative:** NH<sub>4</sub> salt

**CAS Registry Number:** 16675-33-5

**Physical Description:** Cryst. (MeOH aq.)

**Melting Point:** Mp 172-176°

**>>Derivative:** Di-Et ester

**CAS Registry Number:** 3518-88-5

**Molecular Formula:** C<sub>10</sub>H<sub>19</sub>NO<sub>4</sub>

**Molecular Weight:** 217.264

**Accurate Mass:** 217.131409

**Percentage Composition:** C 55.28%; H 8.81%; N 6.45%; O 29.46%

**Boiling Point:** Bp<sub>0.2</sub> 112-114°

**>>Derivative:** Di-Et ester, *N*-Ac

**Molecular Formula:** C<sub>12</sub>H<sub>21</sub>NO<sub>5</sub>

**Molecular Weight:** 259.302

**Accurate Mass:** 259.141974

**Percentage Composition:** C 55.58%; H 8.16%; N 5.40%; O 30.85%

**Boiling Point:** Bp<sub>5</sub> 183-185°

**>>Derivative:** Di-Et ester, *N*-benzoyl

**Molecular Formula:** C<sub>17</sub>H<sub>23</sub>NO<sub>5</sub>

**Molecular Weight:** 321.372

**Accurate Mass:** 321.157624

**Percentage Composition:** C 63.54%; H 7.21%; N 4.36%; O 24.89%

**Boiling Point:** Bp<sub>0.4</sub> 196-198°

**>>Derivative:** Di-Et ester, *N*-benzoyl; hydrochloride

**Physical Description:** Cryst. (EtOH/Et<sub>2</sub>O)

**Melting Point:** Mp 79.5-80.5°

**>>Derivative:** Dinitrile

**Synonym(s):** 3,3'-Iminobispropanenitrile, 9CI. 3,3'-Iminodipropionitrile. Bis(2-cyanoethyl)amine

**CAS Registry Number:** 111-94-4

**Molecular Formula:** C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>

**Molecular Weight:** 123.157

**Accurate Mass:** 123.079647

**Percentage Composition:** C 58.52%; H 7.37%; N 34.12%

**Boiling Point:** Bp<sub>1</sub> 134-135°

**Density:** d<sub>25</sub> 1.463

**Hazard & Toxicity:** May explode on prolonged storage in closed containers. Eye irritant. LD<sub>50</sub> (rat, orl) 2700 mg/kg. Exp. reprod. and teratogenic effects

**Aldrich:** 31730-6

**Rare Chemicals Library:** S37952-2