>>**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

$HOOCCH_2CH_2NHCH_2CH_2COOH$

Molecular Formula: $C_6H_{11}NO_4$
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: pK_a 4.2

>>**Derivative:** NH_4 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: $C_{10}H_{19}NO_4$
Molecular Weight: 217.264
Accurate Mass: 217.131409
Percentage Composition: C 55.28%; H 8.81%; N 6.45%; O 29.46%
Boiling Point: $Bp_{0.2}$ 112-114°

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

Molecular Formula: $C_{12}H_{21}NO_5$
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_5 183-185°

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

Molecular Formula: $C_{17}H_{23}NO_5$
Molecular Weight: 321.372
Accurate Mass: 321.157624
Percentage Composition: C 63.54%; H 7.21%; N 4.36%; O 24.89%
Boiling Point: $Bp_{0.4}$ 196-198°

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

Physical Description: Cryst. ($EtOH/Et_2O$)
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: $C_6H_9N_3$
Molecular Weight: 123.157
Accurate Mass: 123.079647
Percentage Composition: C 58.52%; H 7.37%; N 34.12%
Boiling Point: Bp_1 134-135°
Density: d_{25} 1.463
Hazard & Toxicity: May explode on prolonged storage in closed containers. Eye irritant. LD_{50} (rat, orl) 2700 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: 31730-6
Rare Chemicals Library: S37952-2