



>>Entry Name: Aminopropanedioic acid, 9CI

Synonym(s): Aminomalonic acid

CAS Registry Number: 1068-84-4

Related CAS Registry Numbers(s): 6829-40-9 13433-00-6 16115-80-3 104235-47-4 106308-25-2 114495-68-0 129365-73-7

$\text{H}_2\text{NCH}(\text{COOH})_2$

Molecular Formula: $\text{C}_3\text{H}_5\text{NO}_4$

Molecular Weight: 119.077

Accurate Mass: 119.021859

Percentage Composition: C 30.26%; H 4.23%; N 11.76%; O 53.74%

Physical Description: Prisms + $\text{1H}_2\text{O}$

Melting Point: Mp 109 dec.°

Solubility: Spar. sol. EtOH

pKa Value: $\text{p}K_{\text{a}1}$ 3.32; $\text{p}K_{\text{a}2}$ 9.83 (20°)

Other Data: Decarboxylates on heating

>>Derivative: Hydrochloride

CAS Registry Number: 117975-93-6

Physical Description: Needles (Me_2CO)

Melting Point: Mp 162 dec.°

>>Derivative: Di-Me ester

CAS Registry Number: 53704-09-9

Molecular Formula: $\text{C}_5\text{H}_9\text{NO}_4$

Molecular Weight: 147.13

Accurate Mass: 147.053159

Percentage Composition: C 40.82%; H 6.17%; N 9.52%; O 43.50%

Physical Description: Liq.

Boiling Point: $\text{Bp}_{4.5}$ 92°

>>Derivative: Di-Me ester; hydrochloride

CAS Registry Number: 16115-80-3

Physical Description: Leaflets ($\text{MeOH/Et}_2\text{O}$)

Melting Point: Mp 159° (152°)

Aldrich: 39154-9

Fluka: 8365

>>Derivative: Di-Et ester

CAS Registry Number: 6829-40-9

Molecular Formula: $\text{C}_7\text{H}_{13}\text{NO}_4$

Molecular Weight: 175.184

Accurate Mass: 175.084459

Percentage Composition: C 47.99%; H 7.48%; N 8.00%; O 36.53%

Physical Description: Oil

Boiling Point: Bp_{16} 122-123°. $\text{Bp}_{1.5}$ 80-81°

Refractive Index: n_{D}^{16} 1.4353

>>Derivative: Di-Et ester; hydrochloride

CAS Registry Number: 13433-00-6

Physical Description: Cryst. ($\text{EtOH/Et}_2\text{O}$)

Melting Point: Mp 164-165°

Aldrich: D8758-9

Fluka: 8360

Sigma: D7144