



>>Entry Name: Creatine

Synonym(s): *N*-(Aminoiminomethyl)-*N*-methylglycine, 9Cl. Methylguanidinoacetic acid

CAS Registry Number: 57-00-1

HN=C(NH₂)NMeCH₂COOH

Molecular Formula: C₄H₉N₃O₂

Molecular Weight: 131.134

Accurate Mass: 131.069477

Percentage Composition: C 36.64%; H 6.92%; N 32.04%; O 24.40%

Biological Source: Constit. of blood, muscle, flesh, etc.

Physical Description: Prisms + 1H₂O

Melting Point: Mp 303°

Solubility: Mod. sol. hot H₂O, spar. sol. EtOH, insol. Et₂O

Aldrich: 29119-6

Fluka: 27890

Sigma: C4005

>>Derivative: Hydrate

CAS Registry Number: 6020-87-7

Melting Point: Mp 292 dec.°

Aldrich: 85524-3

Fluka: 27900

Sigma: C3630

>>Derivative: Hydrobromide

CAS Registry Number: 15366-30-0

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 150-151°

>>Derivative: Picrate

Physical Description: Needles (H₂O)

Melting Point: Mp 218-220°

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

Molecular Formula: C₈H₁₃N₃O₄

Molecular Weight: 215.208

Accurate Mass: 215.090607

Percentage Composition: C 44.65%; H 6.09%; N 19.53%; O 29.74%

Physical Description: Needles (EtOH)

Melting Point: Mp 165°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1280B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 785B, (*ir*)

Steudel, H., *Z. Physiol. Chem.*, 1921, **112**, 54, (*synth*)

King, H., *J.C.S.*, 1930, 2374, (*synth*)

Yoshizaki, K. *et al.*, *Biochim. Biophys. Acta*, 1981, **678**, 283, (*pmr*)

Tsuchiya, M. *et al.*, *Int. J. Mass Spectrom. Ion Phys.*, 1983, **46**, 355, (*ms*)