



>>Entry Name: 2-Amino-2-propenoic acid, 9CI

Synonym(s): 2-Aminoacrylic acid, 8CI. Dehydroalanine

CAS Registry Number: 1948-56-7

$\text{H}_2\text{C}=\text{C}(\text{NH}_2)\text{COOH}$

Molecular Formula: $\text{C}_3\text{H}_5\text{NO}_2$

Molecular Weight: 87.078

Accurate Mass: 87.032029

Percentage Composition: C 41.38%; H 5.79%; N 16.09%; O 36.75%

Biological Source: Present in wool and in subtilin from *Staphylococcus aureus*

>>Derivative: N-Ac

CAS Registry Number: 5429-56-1

Molecular Formula: $\text{C}_5\text{H}_7\text{NO}_3$

Molecular Weight: 129.115

Accurate Mass: 129.042594

Percentage Composition: C 46.51%; H 5.46%; N 10.85%; O 37.17%

Melting Point: Mp 204 (185-186°) dec.°

Other Data: Undergoes radical polym.

Aldrich: A140-1

Fluka: 190

Sigma: A3520

>>Derivative: N-Ac, Me ester

Synonym(s): Methyl 2-acetamidoacrylate

CAS Registry Number: 35356-70-8

Molecular Formula: $\text{C}_6\text{H}_9\text{NO}_3$

Molecular Weight: 143.142

Accurate Mass: 143.058244

Percentage Composition: C 50.35%; H 6.34%; N 9.79%; O 33.53%

Physical Description: Cryst. (petrol or pentane)

Melting Point: Mp 52-54° (50-52°)

Boiling Point: Bp₈ 104°

>>Derivative: Nitrile

Synonym(s): 2-Amino-2-propenenitrile, 9CI. 1-Amino-1-cyanoethylene

CAS Registry Number: 69245-10-9

Molecular Formula: $\text{C}_3\text{H}_4\text{N}_2$

Molecular Weight: 68.078

Accurate Mass: 68.037448

Percentage Composition: C 52.93%; H 5.92%; N 41.15%

Use/Importance: Probable prebiotic intermediate

Other Data: Unstable, obt. in soln.

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 542D, (*ir*, *Ac*)

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 847B, (*nmr*)

Rothstein, E., *J.C.S.*, 1949, 1968, (*synth*)

Gross, E. *et al.*, *J.A.C.S.*, 1967, **89**, 2791, (*isol*)

Kolar, A.J. *et al.*, *Synthesis*, 1977, 457-459, (*N-Ac Me ester*)

Seiler, P. *et al.*, *Helv. Chim. Acta*, 1985, **68**, 2093, (*cryst struct*, *nitrile*)

Nelson, G. *et al.*, *Macromol. Synth.*, 1985, **9**, 89, (*polym*, *Ac*)

Bueno, M.P. *et al.*, *Can. J. Chem.*, 1987, **65**, 2182-2186, (*N-Ac Me ester*)

Eschenmoser, A. *et al.*, *Helv. Chim. Acta*, 1987, **70**, 1115; 1990, **73**, 1373, (*nitrile*)

Jähnisch, K. *et al.*, *Synthesis*, 1992, 1211, (*nitrile*, *synth*, *pmr*, *cmr*)

Leroy, C. *et al.*, *Tetrahedron*, 1994, **50**, 13135-13144, (*N-Ac Me ester*)