



>>Entry Name: 4-Amino-2-butenic acid, 9CI

Synonym(s): 4-Aminocrotonic acid

CAS Registry Number: 25747-40-4

$\text{H}_2\text{NCH}_2\text{CH}=\text{CHCOOH}$

Molecular Formula: $\text{C}_4\text{H}_7\text{NO}_2$

Molecular Weight: 101.105

Accurate Mass: 101.047679

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

>>Variant: (*E*)-form

CAS Registry Number: 38090-53-8

Molecular Formula: $\text{C}_4\text{H}_7\text{NO}_2$

Molecular Weight: 101.105

Accurate Mass: 101.047679

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

Use/Importance: Neurochemical transmission inhibitor

Physical Description: Prisms (EtOH)

Melting Point: Mp 164 dec.°

Solubility: Sol. H_2O

>>Derivative: *N*-Tri-Me

>>Variant: (ξ)-form

Molecular Formula: $\text{C}_4\text{H}_7\text{NO}_2$

Molecular Weight: 101.105

Accurate Mass: 101.047679

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

>>Derivative: *N*-Ac

Synonym(s): 4-(Acetylamino)-2-butenic acid, 9CI

CAS Registry Number: 64120-63-4

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%

Source/Synthesis: Metab. of *Fusarium graminearum*

Physical Description: Cryst. (MeOH/CHCl_3)

Melting Point: Mp 140°

References:

Balenovic, K. *et al.*, *J.O.C.*, 1954, **19**, 1589, (*synth*)

Jones, G.P. *et al.*, *J.C.S. Perkin 2*, 1975, 1059, (*cryst struct*)

Vesonder, R.F. *et al.*, *Phytochemistry*, 1977, **16**, 1296, (*deriv, isol*)

Allan, R.D. *et al.*, *Aust. J. Chem.*, 1978, **31**, 2283, (*synth*)