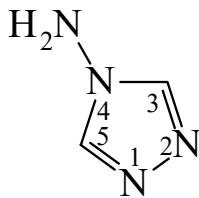




>>Entry Name: 4-Amino-1,2,4-triazole

Synonym(s): 4H-1,2,4-Triazol-4-amine, 9CI



CAS Registry Number: 584-13-4

Related CAS Registry Numbers(s): 10495-63-3

Molecular Formula: C₂H₄N₄

Molecular Weight: 84.08

Accurate Mass: 84.043596

Percentage Composition: C 28.57%; H 4.79%; N 66.63%

Physical Description: Hygroscopic cryst. (EtOH or CHCl₃)

Melting Point: Mp 82-83°

pKa Value: pK_a 3.23

Aldrich: A8180-3

Fluka: 9550

>>Derivative: Hydrochloride

CAS Registry Number: 25545-88-4

Physical Description: Cryst. (EtOH)

Melting Point: Mp 153°

Rare Chemicals Library: S35789-8

>>Derivative: N-Formyl

Molecular Formula: C₃H₄N₄O

Molecular Weight: 112.091

Accurate Mass: 112.038511

Percentage Composition: C 32.15%; H 3.60%; N 49.98%; O 14.27%

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 117°

>>Derivative: N-Benzylidene

Molecular Formula: C₉H₈N₄

Molecular Weight: 172.189

Accurate Mass: 172.074896

Percentage Composition: C 62.78%; H 4.68%; N 32.54%

Melting Point: Mp 169-170°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 627C, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 497D, (*nmr*)

Org. Synth., 1944, **24**, 12, (*synth*)

Buckley, G.D. *et al.*, *J.C.S.*, 1949, 1156, (*deriv*)

Ratz, R.F.W. *et al.*, *J.O.C.*, 1958, **23**, 1931, (*synth*)

Kost, D.N., *Zh. Obshch. Khim.*, 1958, **28**, 2773, (*synth*)