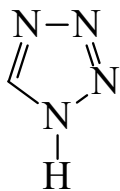




>>Entry Name: Tetrazole
Synonym(s): Tetraazacyclopentadiene



1*H*-form

CAS Registry Number: 288-94-8

Molecular Formula: CH₂N₄
Molecular Weight: 70.054
Accurate Mass: 70.027946
Percentage Composition: C 17.15%; H 2.88%; N 79.98%
Physical Description: Plates (EtOH)
Melting Point: Mp 156°
Solubility: Sol. H₂O, EtOH; spar. sol. Et₂O, C₆H₆
pKa Value: p*K*_a 4.89
Other Data: Sublimes. Dimorphous (monoclinic acid triclinic forms)
Hazard & Toxicity: Salts are explosive when shocked or heated. Explodes above Mp

Aldrich: 15569-1
Fluka: 88185
Sigma: T7641

>>Variant: 1*H*-form

Molecular Formula: CH₂N₄
Molecular Weight: 70.054
Accurate Mass: 70.027946
Percentage Composition: C 17.15%; H 2.88%; N 79.98%

>>Derivative: 1-*N*-Ac

CAS Registry Number: 21565-41-3
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%
Melting Point: Mp 58-59°

>>Derivative: 1-*N*-Benzoyl

CAS Registry Number: 59921-48-1
Molecular Formula: C₈H₆N₄O
Molecular Weight: 174.162
Accurate Mass: 174.054161
Percentage Composition: C 55.17%; H 3.47%; N 32.17%; O 9.19%
Source/Synthesis: Prepared *in situ*
Use/Importance: Mild benzoylating agent for nucleosides

>>Derivative: 1-*N*-Me

Synonym(s): 1-Methyl-1*H*-tetrazole, 9Cl. 1-Methyl-1,2,3,4-tetrazole

CAS Registry Number: 16681-77-9
Molecular Formula: C₂H₄N₄
Molecular Weight: 84.08
Accurate Mass: 84.043596
Percentage Composition: C 28.57%; H 4.79%; N 66.63%
Physical Description: Prisms
Melting Point: Mp 36-37°
Boiling Point: Bp₅ 110°