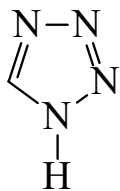




>>Entry Name: Tetrazole

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°