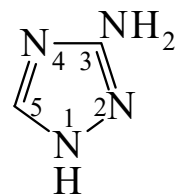




>>>Entry Name: 3(5)-Amino-1,2,4-triazole

Synonym(s): 1*H*-1,2,4-Triazol-3-amine, 9CI. Amizol. Amitrole, ANSI, BSI, ISO, WSSA. Aminotriazole. ATA, JMAF. Weedazol



CAS Registry Number: 61-82-5

Molecular Formula: C₂H₄N₄

Molecular Weight: 84.08

Accurate Mass: 84.043596

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

Use/Importance: Non-selective herbicide. Used for detn. of tryptophan in proteins

Physical Description: Cryst. (H₂O, EtOH or EtOAc)

Melting Point: Mp 159°

pKa Value: pK_{a1} 4.04; pK_{a2} 11.08 (20°)

Hazard & Toxicity: Possible human carcinogen. LD₅₀ (rat, orl) 1100 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects

Aldrich: A8160-9

Fluka: 9540

Sigma: A4383

>>>Derivative: Hydrochloride

Physical Description: Cryst. (EtOH)

Melting Point: Mp 153°

>>>Derivative: 3-*N*-Ac

CAS Registry Number: 5295-23-8

Molecular Formula: C₄H₆N₄O

Molecular Weight: 126.118

Accurate Mass: 126.054161

Percentage Composition: C 38.09%; H 4.80%; N 44.42%; O 12.69%

Melting Point: Mp 295-300 dec.°

Rare Chemicals Library: S56577-6

>>>Derivative: 3-*N*-(2-Hydroxybenzoyl)

Synonym(s): 2-Hydroxy-*N*-1*H*-1,2,4-triazol-3-ylbenzamide, 9CI. 3-Salicylamido-1,2,4-triazole

CAS Registry Number: 36411-52-6

Molecular Formula: C₉H₈N₄O₂

Molecular Weight: 204.188

Accurate Mass: 204.064726

Percentage Composition: C 52.94%; H 3.95%; N 27.44%; O 15.67%

Use/Importance: Antioxidant for polymers, esp. polypropylene in the presence of Cu

>>>Variant: 1*H*-form

Molecular Formula: C₂H₄N₄

Molecular Weight: 84.08

Accurate Mass: 84.043596

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

>>>Derivative: 1-Ph

Synonym(s): 3-Amino-1-phenyl-1,2,4-triazole. 1-Phenyl-1*H*-1,2,4-triazol-3-amine

Molecular Formula: C₈H₈N₄

Molecular Weight: 160.178

Accurate Mass: 160.074896

Percentage Composition: C 59.99%; H 5.03%; N 34.98%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 150°