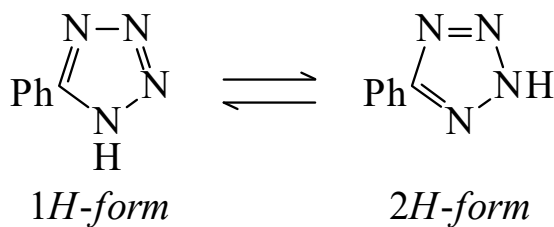




>>Entry Name: 5-Phenyltetrazole



Molecular Formula: C₇H₆N₄

Molecular Weight: 146.151

Accurate Mass: 146.059246

Percentage Composition: C 57.53%; H 4.14%; N 38.33%

Use/Importance: Blowing agent for polymers

Hazard & Toxicity: Synth. may be hazardous, explodes on attempted dist.

>>Variant: 1*H*-form

CAS Registry Number: 18039-42-4

Molecular Formula: C₇H₆N₄

Molecular Weight: 146.151

Accurate Mass: 146.059246

Percentage Composition: C 57.53%; H 4.14%; N 38.33%

Physical Description: Cryst. (EtOH or dioxan)

Melting Point: Mp 217-218° (212.5-213 dec.)

pKa Value: p*K*_a 4.54

Other Data: Major tautomer in solvents such as DMSO

Aldrich: 34774-4

Rare Chemicals Library: S57793-6

>>Derivative: *N*-Hydroxy

CAS Registry Number: 55513-24-1

Molecular Formula: C₇H₆N₄O

Molecular Weight: 162.151

Accurate Mass: 162.054161

Percentage Composition: C 51.85%; H 3.73%; N 34.55%; O 9.87%

Melting Point: Mp 151-152 dec.°

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-5-phenyl-1*H*-tetrazole

CAS Registry Number: 20743-50-4

Molecular Formula: C₈H₈N₄

Molecular Weight: 160.178

Accurate Mass: 160.074896

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

Physical Description: Needles (petrol/C₆H₆)

Melting Point: Mp 103-104°

>>Derivative: *N*-Et

Synonym(s): 1-Ethyl-5-phenyl-1*H*-tetrazole

CAS Registry Number: 24433-71-4

Molecular Formula: C₉H₁₀N₄

Molecular Weight: 174.205

Accurate Mass: 174.090546

Percentage Composition: C 62.05%; H 5.79%; N 32.16%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 70-71°