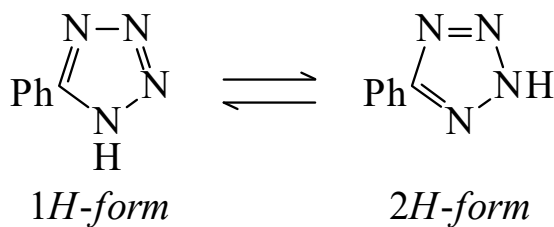




>>Entry Name: 5-Phenyltetrazole



**Molecular Formula:** C<sub>7</sub>H<sub>6</sub>N<sub>4</sub>

**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:** C<sub>7</sub>H<sub>6</sub>N<sub>4</sub>

**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*<sub>a</sub> 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:** C<sub>7</sub>H<sub>6</sub>N<sub>4</sub>O

**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:** C<sub>8</sub>H<sub>8</sub>N<sub>4</sub>

**Molecular Weight:** 160.178

**Accurate Mass:** 160.074896

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

**Physical Description:** Needles (petrol/C<sub>6</sub>H<sub>6</sub>)

**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:** C<sub>9</sub>H<sub>10</sub>N<sub>4</sub>

**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°