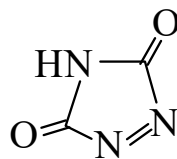




>>Entry Name: **3*H*-1,2,4-Triazole-3,5(4*H*)-dione**, 9CI

Synonym(s): 1,2,4-Triazoline-3,5-dione



CAS Registry Number: 4019-43-6

Molecular Formula: C₂HN₃O₂

Molecular Weight: 99.049

Accurate Mass: 99.006877

Percentage Composition: C 24.25%; H 1.02%; N 42.42%; O 32.31%

Use/Importance: Synthon, reactive dienophile

Physical Description: Red

Other Data: λ_{max} 504 sh, 520, 540 and 563 nm

>>Derivative: 4-Me

Synonym(s): 4-Methyl-3*H*-1,2,4-triazole-3,5(4*H*)-dione. MTAD. 4-Methyl-1,2,4-triazoline-3,5-dione

CAS Registry Number: 13274-43-6

Molecular Formula: C₃H₃N₃O₂

Molecular Weight: 113.076

Accurate Mass: 113.022527

Percentage Composition: C 31.87%; H 2.67%; N 37.16%; O 28.30%

Use/Importance: Extremely reactive dienophile. Derivatisation reagent for gc-ms of conjugated dienes

Physical Description: Bright-pink needles by subl.

Melting Point: Mp 103-104°

Boiling Point: Subl._{0,1} 50°

Aldrich: 32912-6

>>Derivative: 4-*tert*-Butyl

Synonym(s): 4-*tert*-Butyl-1,2,4-triazoline-3,5-dione

CAS Registry Number: 35403-69-1

Molecular Formula: C₆H₉N₃O₂

Molecular Weight: 155.156

Accurate Mass: 155.069477

Percentage Composition: C 46.45%; H 5.85%; N 27.08%; O 20.62%

Melting Point: Mp 119°

Boiling Point: Subl._{0,1} 50°

>>Derivative: 4-Ph

Synonym(s): 4-Phenyl-1,2,4-triazole-3,5-dione

CAS Registry Number: 4233-33-4

Molecular Formula: C₈H₅N₃O₂

Molecular Weight: 175.146

Accurate Mass: 175.038177

Percentage Composition: C 54.86%; H 2.88%; N 23.99%; O 18.27%

Use/Importance: Dienophile. Spin trap for carbon- and metal- centred radicals

Physical Description: Red needles

Melting Point: Mp 170-175 dec.°

Aldrich: 28099-2

Fluka: 79225

>>Derivative: 4-(4-Nitrophenyl)

Synonym(s): 4-(4-Nitrophenyl)-1,2,4-triazole-3,5-dione

CAS Registry Number: 13274-75-4

Molecular Formula: C₈H₄N₄O₄

Molecular Weight: 220.144

Accurate Mass: 220.023256

Percentage Composition: C 43.65%; H 1.83%; N 25.45%; O 29.07%

Melting Point: Mp 130°

References: