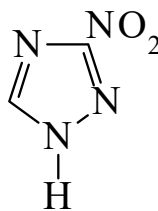




>>Entry Name: 3(5)-Nitro-1,2,4-triazole



**CAS Registry Number:** 24807-55-4

**Related CAS Registry Numbers(s):** 36899-13-5 50738-31-3 76216-87-0 76216-88-1 79443-15-5 79443-22-4 91039-58-6

**Molecular Formula:** C<sub>2</sub>H<sub>2</sub>N<sub>4</sub>O<sub>2</sub>

**Molecular Weight:** 114.063

**Accurate Mass:** 114.017776

**Percentage Composition:** C 21.06%; H 1.77%; N 49.12%; O 28.05%

**Physical Description:** Cryst. (MeOH), pale yellow prisms (H<sub>2</sub>O)

**Melting Point:** Mp 215-216 dec.° (208-210°)

**Aldrich:** 24179-2

**Fluka:** 74085

**Sigma:** N3759

>>Derivative: N<sup>1</sup>-4-Methylbenzenesulfonyl

**CAS Registry Number:** 77451-51-5

**Use/Importance:** Coupling reagent in oligonucleotide synth.

**Melting Point:** Mp 133-135°

**Other Data:** Moisture sensitive

**Aldrich:** 24417-1

**Sigma:** T6643

>>Derivative: N<sup>1</sup>-(2,4,6-Trimethylbenzenesulfonyl)

**Molecular Formula:** C<sub>11</sub>H<sub>12</sub>N<sub>4</sub>O<sub>4</sub>S

**Molecular Weight:** 296.306

**Accurate Mass:** 296.057926

**Percentage Composition:** C 44.59%; H 4.08%; N 18.91%; O 21.60%; S 10.82%

**Use/Importance:** Coupling agent for oligonucleotide synth

**Physical Description:** Cryst. (C<sub>6</sub>H<sub>6</sub>)

**Melting Point:** Mp 130-132°

>>Derivative: N<sup>1</sup>-(2,4,6-Triisopropylbenzenesulfonyl)

**CAS Registry Number:** 73118-37-3

**Molecular Formula:** C<sub>17</sub>H<sub>24</sub>N<sub>4</sub>O<sub>4</sub>S

**Molecular Weight:** 380.467

**Accurate Mass:** 380.151826

**Percentage Composition:** C 53.67%; H 6.36%; N 14.73%; O 16.82%; S 8.43%

**Use/Importance:** Coupling reagent for oligonucleotide synth.

**Physical Description:** Cryst. (CHCl<sub>3</sub>/petrol)

**Melting Point:** Mp 128-130°

#### References:

*Aldrich Library of NMR Spectra, 2nd edn.*, 1983, **2**, 497C, (*nmr*)

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Brown, E.J., *Aust. J. Chem.*, 1969, **22**, 2251, (*synth*)

Closset, J.L. *et al.*, *Bull. Soc. Chim. Belg.*, 1975, **84**, 1023, (*ir, ms, cmr, cryst struct*)

De Rooij, J.F.M. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1979, **98**, 537, (*2,4,6-triisopropylbenzenesulfonyl*)

Jones, S.S. *et al.*, *Tetrahedron*, 1980, **36**, 3075, (*synth, allylbenzenesulfonyl derivs*)