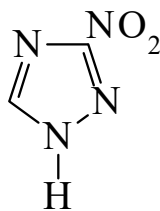




>>Entry Name: 3(5)-Nitro-1,2,4-triazole



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: C₂H₂N₄O₂

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 (H₂O)

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

Aldrich: 24179-2

Fluka: 74085

Sigma: N3759

>>Derivative: N¹-4-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: N¹-(2,4,6-Trimethylbenzenesulfonyl)

Molecular Formula: C₁₁H₁₂N₄O₄S

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. (C₆H₆)

Melting Point: Mp 130-132°

>>Derivative: N¹-(2,4,6-Triisopropylbenzenesulfonyl)

CAS Registry Number: 73118-37-3

Molecular Formula: C₁₇H₂₄N₄O₄S

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. (CHCl₃/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*)