



>>Entry Name: **2-(Hydroxymethyl)-2-nitro-1,3-propanediol, 9CI**

Synonym(s): Tris(hydroxymethyl)nitromethane. Trimethylolnitromethane. Nitroisobutyl glycerol. Tris nitro

CAS Registry Number: 126-11-4



Molecular Formula: C₄H₉NO₅

Molecular Weight: 151.119

Accurate Mass: 151.048074

Percentage Composition: C 31.79%; H 6.00%; N 9.27%; O 52.94%

Use/Importance: Bactericide. Also acts as a nitroxyl group reagent

Physical Description: Cryst. (EtOAc/C₆H₆)

Melting Point: Mp 214° (pure)

Solubility: Spar. sol. C₆H₆; sol. H₂O

Calculated Log P Data: Log P -2.82 (calc)

Other Data: Several polyesters have been synth.

Hazard & Toxicity: LD₅₀ (rat, orl) 1900 mg/kg

Aldrich: 10818-9

Fluka: 93360

Rare Chemicals Library: S42914-7

References:

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Kowalik, R. *et al.*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1969, **17**, 209; *CA*, **71**, 70675p, (*synth*)

Bennett, E.O., *CA*, 1974, **81**, 93733b, (*use*)

Janzen, E.G. *et al.*, *J.O.C.*, 1978, **43**, 1900, (*use*)

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Dewey, R.H. *et al.*, *Kirk-Othmer Encycl. Chem. Technol.*, 3rd edn., Wiley, 1978, **15**, 910, (*rev*)

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Gowda, D.S.S. *et al.*, *J. Chem. Phys.*, 1982, **77**, 4671, (*cryst struct*)

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