



>>Entry Name: **1,3-Diamino-2-propanol**, 9CI

Synonym(s): 2-Hydroxytrimethylenediamine

CAS Registry Number: 616-29-5

$\text{H}_2\text{NCH}_2\text{CH}(\text{OH})\text{CH}_2\text{NH}_2$

Molecular Formula: $\text{C}_3\text{H}_{10}\text{N}_2\text{O}$

Molecular Weight: 90.125

Accurate Mass: 90.079313

Percentage Composition: C 39.98%; H 11.18%; N 31.08%; O 17.75%

Melting Point: Mp 42°

Boiling Point: Bp 235°. Bp₂₀ 145-165°

Hazard & Toxicity: Highly flammable, fl. p. -3°

Aldrich: D1860-9

Fluka: 33262

Sigma: D7889

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 34989-00-9

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 184.5°

>>Derivative: Picrate

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 236-237.2°

>>Derivative: N-Tetra-Me

CAS Registry Number: 5966-51-8

Molecular Formula: $\text{C}_7\text{H}_{18}\text{N}_2\text{O}$

Molecular Weight: 146.232

Accurate Mass: 146.141913

Percentage Composition: C 57.50%; H 12.41%; N 19.16%; O 10.94%

Boiling Point: Bp₁₇ 80-82°

Aldrich: B4298-5

>>Derivative: N-Hexa-Me, diiodide

Synonym(s): 2-Hydroxy-N,N,N',N',N'-hexamethyl-1,3-propanediaminium diiodide, 9CI. (2-Hydroxytrimethylene)bis(trimethylammonium)diiodide, 8CI. **Prolonium iodide**, INN. Entodon. Esiodine. Iodoxil. Propiodal. Tensodex. Endoiodin. Iodisan. Intraiodine. Many other names

CAS Registry Number: 123-47-7

Molecular Formula: $\text{C}_9\text{H}_{24}\text{I}_2\text{N}_2\text{O}$

Molecular Weight: 430.11

Accurate Mass: 429.997809

Percentage Composition: C 25.13%; H 5.62%; I 59.01%; N 6.51%; O 3.72%

Biological Use/Importance: Spasmolytic, hypertensive agent; iodine source

Melting Point: Mp 275 dec.°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 553A, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 349B; 350B, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 438D; 439B, (ir)

Gödeckemeyer, C., *Ber.*, 1888, **21**, 2684, (synth)

Gabriel, S., *Ber.*, 1889, **22**, 224

U.S. Pat., 1925, 1 526 627; *CA*, **19**, 1757, (*Prolonium*)

Gibson, C.S. *et al.*, *J.C.S.*, 1942, 163, (*deriv*)

Roushdi, I.M. *et al.*, *CA*, 1947, **41**, 6188c, (*Prolonium*)

Van der Werf, C.A. *et al.*, *J.A.C.S.*, 1954, **76**, 1231, (*synth*)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., *Akademie-Verlag*, 1987, 1386

Martindale, The Extra Pharmacopoeia, 30th edn., *Pharmaceutical Press*, 1993, 973

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., *Van Nostrand Reinhold*, 1979, 542