



>>Entry Name: **1,1'-Iminobis-2-propanol**, 9CI

Synonym(s): Diisopropanolamine. DIPA

CAS Registry Number: 110-97-4

$\text{H}_3\text{CCH}(\text{OH})\text{CH}_2\text{NHCH}_2\text{CH}(\text{OH})\text{CH}_3$

Molecular Formula: $\text{C}_6\text{H}_{15}\text{NO}_2$

Molecular Weight: 133.19

Accurate Mass: 133.110279

Percentage Composition: C 54.11%; H 11.35%; N 10.52%; O 24.02%

Physical Description: Cryst.

Melting Point: Mp 44.5-45.5°

Boiling Point: Bp₇₄₅ 249-250°

Aldrich: 13301-9

Fluka: 14960

>>Derivative: Hydrochloride

CAS Registry Number: 58901-13-6

Physical Description: Cryst. (2-propanol/AcOH)

Melting Point: Mp 79-82°

>>Derivative: Picrate

Physical Description: Prisms (EtOH)

Melting Point: Mp 130-136°

>>Derivative: Bis(4-nitrobenzoyl)

CAS Registry Number: 19207-78-4

Molecular Formula: $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O}_8$

Molecular Weight: 431.401

Percentage Composition: C 55.68%; H 4.91%; N 9.74%; O 29.67%

Physical Description: Cryst. (2-propanol) (as hydrochloride)

Melting Point: Mp 190-192 dec.°

Other Data: CAS no. refers to hydrochloride

>>Derivative: *N*-Nitroso

Synonym(s): 2,2'-Dihydroxy-di-*n*-propylnitrosamine. *N*-Nitrosobis(2-hydroxypropyl)amine. Diisopropanolnitrosamine

CAS Registry Number: 53609-64-6

Molecular Formula: $\text{C}_6\text{H}_{14}\text{N}_2\text{O}_3$

Molecular Weight: 162.188

Accurate Mass: 162.100443

Percentage Composition: C 44.43%; H 8.70%; N 17.27%; O 29.59%

Boiling Point: Bp_{0.01} 95°

Refractive Index: n_D^{21} 1.4826

Hazard & Toxicity: Carcinogen

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 341C, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 544C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 431C, (*ir*)

Krasuskis, K., *J. Gen. Chem. USSR (Engl. Transl.)*, 1936, **6**, 460, (*synth*)

Kretov, A.E. *et al.*, *Zh. Obshch. Khim.*, 1962, **32**, 471; *CA*, **58**, 1337d, (*synth*)

Krueger, F.W. *et al.*, *Naturwissenschaften*, 1974, **61**, 328, (*N-nitroso*, *synth*, *tox*)

Mori, Y. *et al.*, *Carcinogenesis (London)*, 1984, **5**, 1443-1447, (*N-nitroso*)

Yamamoto, K. *et al.*, *Cancer Lett. (Shannon, Irel.)*, 1989, **45**, 221-225, (*N-nitroso*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DNL600