



>>Entry Name: Tris(2-chloroethyl)amine

Synonym(s): 2-Chloro-*N,N*-bis(2-chloroethyl)ethanamine, 9Cl. 2,2',2''-Trichlorotriethylamine, 8Cl. Trimustine, BAN. **Trichlormethine**, INN. Nitrogen Lost. NSC 30211

CAS Registry Number: 555-77-1

$(\text{ClCH}_2\text{CH}_2)_3\text{N}$

Molecular Formula: $\text{C}_6\text{H}_{12}\text{Cl}_3\text{N}$

Molecular Weight: 204.526

Accurate Mass: 203.00353

Percentage Composition: C 35.24%; H 5.91%; Cl 52.00%; N 6.85%

Use/Importance: Chemical warfare agent, biological alkylating agent with mutagenic and cytotoxic activity. Antineoplastic agent

Physical Description: Mobile liq. with faint odour of fish and soap

Boiling Point: Bp_2 98°

Refractive Index: n_D^{25} 1.4925

Calculated Log P Data: Log P 1.66 (calc)

Hazard & Toxicity: Eye irritant, vesicant. LD_{50} (rat, orl) 5 mg/kg. LD_{50} (rat, skn) 2 mg/kg. Exp. carcinogen

>>Derivative: Hydrochloride

Synonym(s): Lekamin. Trillekamin. Trimitan. SK 100. TS 160

CAS Registry Number: 817-09-4

Physical Description: Cryst. (EtOH/ Me_2CO)

Melting Point: Mp 131-132.2°

Hazard & Toxicity: Adverse systemic effects reported when used therapeutically. LD_{50} (rat, ipr) 0.75 mg/kg. Exp. carcinogen. Exp. reprod. effects

Aldrich: T8530-8

>>Derivative: *N*-Oxide

Molecular Formula: $\text{C}_6\text{H}_{12}\text{Cl}_3\text{NO}$

Molecular Weight: 220.525

Accurate Mass: 218.998445

Percentage Composition: C 32.68%; H 5.48%; Cl 48.23%; N 6.35%; O 7.26%

Physical Description: Cryst. (Me_2CO) (as hydrochloride)

Melting Point: Mp 91-92° (hydrochloride)

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 327B, (*hydrochloride*, *ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 283C; **2**, 38B, (*hydrochloride*, *pmr*, *nmr*)

Ward, K., *J.A.C.S.*, 1935, **57**, 914, (*synth*)

Wilson, E. *et al.*, *J.A.C.S.*, 1951, **73**, 3635, (*synth*)

Kimura, E. *et al.*, *Inorg. Chem.*, 1970, **9**, 1183, (*synth*)

IARC Monog., 1975, **9**, 229; *Suppl.* 7, 73, (*rev*, *tox*)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., *Pharmaceutical Press*, 1982, 1874

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, TNF250; TNF500