



>>Entry Name: *N*-[3-(Dimethylamino)propyl]-*N'*-ethylcarbodiimide, 8Cl

ENTRY UNDER REVIEW

Synonym(s): *N'*-(Ethylcarbimidoyl)-*N,N*-dimethyl-1,3-propanediamine, 9Cl

CAS Registry Number: 1892-57-5

Related CAS Registry Numbers(s): 7084-11-9

Me2NCH2CH2CH2N=C=NEt

Molecular Formula: C₈H₁₇N₃

Molecular Weight: 155.242

Accurate Mass: 155.142247

Percentage Composition: C 61.90%; H 11.04%; N 27.07%

Use/Importance: Reagent used in peptide synth. Also reagent (followed by borohydride reduction) for conversion of uronic acids to monosaccharide units

Physical Description: Liq.

Boiling Point: Bp_{0.27} 47-48°

Density: d₄²⁰ 0.89

Refractive Index: n_D²⁵ 1.4582

Fluka: 39391

Other: JBL Scientific (bulk supplier)

>>Derivative: Hydrochloride

CAS Registry Number: 25952-53-8

Extra CAS Registry Numbers(s): 7084-11-9

Physical Description: Cryst. (CH₂Cl₂/EtOH)

Melting Point: Mp 113.5-114.5°

Hazard & Toxicity: LD₅₀ (mus, ivn) 56 mg/kg

Aldrich: 16146-2

Fluka: 3451

Sigma: E7750

Other: JBL Scientific (bulk supplier)

>>Derivative: Methiodide

CAS Registry Number: 22572-40-3

Melting Point: Mp 94-95°

Aldrich: 16534-4

Sigma: E0388

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 729B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 877A, (*ir*)

Kopple, K.D. *et al.*, *J.A.C.S.*, 1962, **84**, 4457, (*use*)

Taylor, R.L. *et al.*, *Biochemistry*, 1972, **11**, 1383; 1973, **12**, 3633, (*use, uronic acids*)

Tenforde, T. *et al.*, *J.O.C.*, 1972, **37**, 3372, (*ir, pmr*)

Org. Synth., *Coll. Vol.*, 5, 1973, 555, (*synth*)

Yavari, I. *et al.*, *J.O.C.*, 1978, **43**, 4689, (*cmr, nmr*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1986, **12**, 199, (*use*)