



>>Entry Name: **Elmustine**, INN

Synonym(s): *N*-(2-Chloroethyl)-*N'*-(2-hydroxyethyl)-*N*-nitrosourea, 9Cl. CNU-ethanol. NSC 29485. HECNU

CAS Registry Number: 60784-46-5

Type of Compound Code(s): XA1950

HOCH₂CH₂NHCON(NO)CH₂CH₂Cl

Molecular Formula: C₅H₁₀ClN₃O₃

Molecular Weight: 195.605

Accurate Mass: 195.041069

Percentage Composition: C 30.70%; H 5.15%; Cl 18.12%; N 21.48%; O 24.54%

Use/Importance: Antineoplastic agent

Melting Point: Mp 56°

Solubility: Sol. H₂O

Calculated Log P Data: Log P 0.08 (calc)

Hazard & Toxicity: Low toxicity compared with Carmustine [DLG43-W](#). LD₅₀ (mus, ipr) 25 mg/kg. Mutagen

>>Derivative: *N'*-Me

CAS Registry Number: 70189-79-6

Type of Compound Code(s): XA1950

Molecular Formula: C₆H₁₂ClN₃O₃

Molecular Weight: 209.632

Accurate Mass: 209.056719

Percentage Composition: C 34.38%; H 5.77%; Cl 16.91%; N 20.04%; O 22.90%

Use/Importance: Possesses antineoplastic props.

Physical Description: Yellow oil

Calculated Log P Data: Log P 0.04 (calc)

References:

- Fiebig, H.H. *et al.*, *Eur. J. Cancer*, 1977, **13**, 937, (*pharmacol*)
Eisenbrand, G. *et al.*, *Dev. Toxicol. Environ. Sci.*, 1980, **8**, 273, (*pharmacol, tox*)
Tsujihara, K. *et al.*, *Chem. Pharm. Bull.*, 1981, **29**, 2509, (*derivs*)
Lown, J.W. *et al.*, *J.O.C.*, 1981, **46**, 5309, (*synth, nmr*)
Lijinsky, W. *et al.*, *J. Cancer Res. Clin. Oncol.*, 1986, **112**, 221, (*synth, pmr, uv, ms, activity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 477
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CHB750