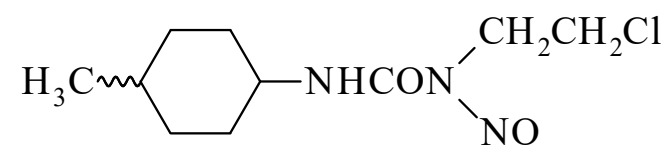




>>Entry Name: Semustine, INN, USAN

Synonym(s): *N*-(2-Chloroethyl)-*N'*-(4-methylcyclohexyl)-*N*-nitrosourea, 9Cl, 8Cl. Methyl CCNU. NSC 95441



CAS Registry Number: 13909-09-6

Molecular Formula: C₁₀H₁₈ClN₃O₂

Molecular Weight: 247.724

Accurate Mass: 247.108754

Percentage Composition: C 48.49%; H 7.32%; Cl 14.31%; N 16.96%; O 12.92%

Use/Importance: Antineoplastic agent

Melting Point: Mp 64 dec.°

Calculated Log P Data: Log P 3.27 (calc)

Other Data: Methyl analogue of Lomustine [FLZ07-B](#)

Hazard & Toxicity: Nephrotoxic effects reported when used therapeutically. LD₅₀ (mus, orl) *ca.* 50 mg/kg. Exp. carcinogenic data

Sigma: S4026

References:

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Lown, J.W. *et al.*, *J.O.C.*, 1981, **46**, 5309, (*synth, N-15 nmr, cmr, bibl*)

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Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 598

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, CHD250