# Semustine

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|---|---|
| **Other names:** | Urea, N-(2-chloroethyl)-N'-(4-methylcyclohexyl)-N-nitroso- |
| | Urea, 1-(2-chloroethyl)-3-(4-methylcyclohexyl)-1-nitroso- |
| | ICIG 1110 |
| | Me-CCNU |
| | Methyl-CCNU |
| | NSC 95441 |
| | 1-(2-Chloroethyl)-3-(4-methyl-cyclohexyl)-1-nitrosourea |
| | N-(2-Chloroethyl)-N'-(4-methylcyclohexyl)-N-nitrosourea |
| | Lomustine, methyl- |
| | NCI-C04955 |
| | 1-(2-Chloroethyl)-1-([(4-methylcyclohexyl)amino]carbonyl)-2-oxohydrazine |
| | Urea, 3-(beta-chloroethyl)-1-(4-methylcyclohexyl)-3-nitroso- |
| **Inchi:** | InChI=1S/C10H18ClN3O2/c1-8-2-4-9(5-3-8)12-10(15)14(13-16)7-6-11/h8-9H,2-7H2,1H3 |
| **InchiKey:** | FVLVBPDQNARYJU-UHFFFAOYSA-N |
| **Formula:** | C10H18ClN3O2 |
| **SMILES:** | CC1CCC(N=C(O)N(CCCl)N=O)CC1 |
| **Mol. weight [g/mol]:** | 247.72 |
| **CAS:** | 13909-09-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -411.95 | kJ/mol | Joback Method |
| hvap | 73.57 | kJ/mol | Joback Method |
| log10ws | -3.16 | | Crippen Method |
| logp | 2.701 | | Crippen Method |
| mcvol | 186.220 | ml/mol | McGowan Method |
| pc | 2331.52 | kPa | Joback Method |
| tb | 725.09 | K | Joback Method |
| tc | 927.73 | K | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13909096&Units=SI |

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |