Urea, N-(2-chloroethyl)-N'-(2,6-dioxo-3-piperidinyl)-N-nit

Other names: N-(2-Chloroethyl)-N'-(2,6-dioxo-3-piperidinyl)-N-nitrosourea
NSC-95,466
NSC-95466
PCNU
Urea, 1-(2-chloroethyl)-3-(2,6-dioxo-3-piperidyl)-1-nitroso-
1-(2-Chloroethyl)-3-(2,6-dioxo-3-piperidyl)-1-nitrosourea
3-(([1-(2-Chloroethyl)-2-oxohydrazino]carbonyl)amino)-2,6-piperidinedione

Inchi: InChI=1S/C8H11ClN4O4/c9-3-4-13(12-17)8(16)10-5-1-2-6(14)11-7(5)15/h5H,1-4H2,(H,1

InchiKey: KHWIRCOLWPNBJP-UHFFFAOYSA-N

Formula: C8H11ClN4O4

SMILES: O=NN(CCCl)C(=O)NC1CCC(=O)NC1=O

Mol. weight [g/mol]: 262.65

CAS: 13909-02-9

Physical Properties

Property code	Value	Unit	Source
hf	-567.23	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	-0.277		Crippen Method
mcvol	171.160	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	803.49	K	Joback Method
tc	1038.72	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13909029&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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