Biuret, 5-(2-chloroethyl)-1-methyl-1-nitroso-

Inchi:	InChI=1S/C5H9ClN4O3/c1-10(9-13)5(12)8-4(11)7-3-2-6/h2-3H2,1H3,(H2,7,8,11,12)
InchiKey:	FTHZEGJUANZMRJ-UHFFFAOYSA-N
Formula:	C5H9ClN4O3
SMILES:	CN(N=O)C(=O)NC(=O)NCCCl
Mol. weight [g/mol]:	208.60
CAS:	13857-11-9

Physical Properties

Property code	Value	Unit	Source
hf	-381.15	kJ/mol	Joback Method
hvap	68.61	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	0.258		Crippen Method
mcvol	138.180	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	635.15	K	Joback Method
tc	830.65	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13857119&Units=SI

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

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