N'-(2-chloroethyl)-n-methoxy-n-methylurea

Inchi: InChI=1S/C5H11ClN2O2/c1-8(10-2)5(9)7-4-3-6/h3-4H2,1-2H3,(H,7,9)
InchiKey: IOAXIRGUNIEWQT-UHFFFAOYSA-N
Formula: C5H11ClN2O2
SMILES: CON(C)C(=O)NCCCl
Mol. weight [g/mol]: 166.61
CAS: 133318-33-9

Physical Properties

Property code	Value	Unit	Source
gf	-54.46	kJ/mol	Joback Method
hf	-286.07	kJ/mol	Joback Method
hfus	23.81	kJ/mol	Joback Method
hvap	48.74	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.428		Crippen Method
mcvol	120.950	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	490.13	K	Joback Method
tc	677.07	K	Joback Method
tf	333.32	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.37	J/mol×K	490.13	Joback Method
cpg	266.43	J/mol×K	521.29	Joback Method
cpg	276.03	J/mol×K	552.44	Joback Method
cpg	285.18	J/mol×K	583.60	Joback Method
cpg	293.88	J/mol×K	614.75	Joback Method
cpg	302.16	J/mol×K	645.91	Joback Method
cpg	310.00	J/mol×K	677.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C133318339&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume