Biurea, 1-(2-chloroethyl)-6-methyl-

Inchi: InChI=1S/C5H11ClN4O2/c1-7-4(11)9-10-5(12)8-3-2-6/h2-3H2,1H3,(H2,7,9,11)(H2,8,10,1
InchiKey: FBEHXFQFBLYAOC-UHFFFAOYSA-N
Formula: C5H11ClN4O2
SMILES: CNC(=O)NNC(=O)NCCCl
Mol. weight [g/mol]: 194.62
CAS: 16813-41-5

Physical Properties

Property code	Value	Unit	Source
gf	79.01	kJ/mol	Joback Method
hf	-173.55	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	70.34	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	-0.632		Crippen Method
mcvol	136.610	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
tb	659.65	K	Joback Method
tc	861.52	K	Joback Method
tf	486.53	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.69	J/mol×K	659.65	Joback Method
cpg	352.78	J/mol×K	693.29	Joback Method
cpg	361.29	J/mol×K	726.94	Joback Method
cpg	369.23	J/mol×K	760.58	Joback Method
cpg	376.63	J/mol×K	794.23	Joback Method
cpg	383.51	J/mol×K	827.87	Joback Method
cpg	389.88	J/mol×K	861.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16813415&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