Urea, 1-(2-chloroethyl)-3-(cyanomethyl)-

Inchi: InChI=1S/C5H8ClN3O/c6-1-3-8-5(10)9-4-2-7/h1,3-4H2,(H2,8,9,10)
InchiKey: JLXBWDRUULBIQN-UHFFFAOYSA-N
Formula: C5H8ClN3O
SMILES: N#CCNC(=O)NCCCl
Mol. weight [g/mol]: 161.59
CAS: 13991-67-8

Physical Properties

Property code	Value	Unit	Source
gf	162.33	kJ/mol	Joback Method
hf	-3.03	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.048		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	607.52	K	Joback Method
tc	815.89	K	Joback Method
tf	396.27	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.60	J/mol×K	607.52	Joback Method
cpg	269.36	J/mol×K	642.25	Joback Method
cpg	276.66	J/mol×K	676.98	Joback Method
cpg	283.49	J/mol×K	711.71	Joback Method
cpg	289.90	J/mol×K	746.44	Joback Method
cpg	295.87	J/mol×K	781.16	Joback Method
cpg	301.44	J/mol×K	815.89	Joback Method

Sources

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=C13991678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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