Acetic acid, 3(2-chloroethyl)ureido-

Inchi: InChI=1S/C5H9ClN2O3/c6-1-2-7-5(11)8-3-4(9)10/h1-3H2,(H,9,10)(H2,7,8,11)
InchiKey: CEDUJPWCSLBKJL-UHFFFAOYSA-N
Formula: C5H9ClN2O3
SMILES: O=C(O)CNC(=O)NCCCl
Mol. weight [g/mol]: 180.59
CAS: 87219-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-236.59	kJ/mol	Joback Method
hf	-432.72	kJ/mol	Joback Method
hfus	30.39	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-0.30		Crippen Method
logp	-0.391		Crippen Method
mcvol	122.520	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	651.49	K	Joback Method
tc	841.41	K	Joback Method
tf	442.03	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.21	J/mol×K	651.49	Joback Method
cpg	304.52	J/mol×K	683.14	Joback Method
cpg	311.39	J/mol×K	714.80	Joback Method
cpg	317.84	J/mol×K	746.45	Joback Method
cpg	323.89	J/mol×K	778.10	Joback Method
cpg	329.54	J/mol×K	809.75	Joback Method
cpg	334.82	J/mol×K	841.41	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=C87219189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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