Glycine, n-[(2-chloroethyl)carbamoyl]-, ethyl ester

Inchi: InChI=1S/C7H13ClN2O3/c1-2-13-6(11)5-10-7(12)9-4-3-8/h2-5H2,1H3,(H2,9,10,12)
InchiKey: RGAPZOUEBKAJOU-UHFFFAOYSA-N
Formula: C7H13ClN2O3
SMILES: CCOC(=O)CNC(=O)NCCCl
Mol. weight [g/mol]: 208.64
CAS: 7145-35-9

Physical Properties

Property code	Value	Unit	Source
gf	-187.93	kJ/mol	Joback Method
hf	-453.99	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	64.33	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.087		Crippen Method
mcvol	150.700	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	627.49	K	Joback Method
tc	821.67	K	Joback Method
tf	425.98	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.77	J/mol×K	627.49	Joback Method
cpg	381.30	J/mol×K	659.85	Joback Method
cpg	391.26	J/mol×K	692.22	Joback Method
cpg	400.67	J/mol×K	724.58	Joback Method
cpg	409.52	J/mol×K	756.94	Joback Method
cpg	417.83	J/mol×K	789.31	Joback Method
cpg	425.61	J/mol×K	821.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7145359&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