DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, propyl ester

Inchi: InChI=1S/C11H20ClNO4/c1-4-7-16-10(14)9(2)13(3)11(15)17-8-5-6-12/h9H,4-8H2,1-3H3
InchiKey: RVUFJTLRBZSEJN-UHFFFAOYSA-N
Formula: C11H20ClNO4
SMILES: CCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 265.73

Physical Properties

Property code	Value	Unit	Source
gf	-329.69	kJ/mol	Joback Method
hf	-713.46	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.025		Crippen Method
mcvol	202.950	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	653.09	K	Joback Method
tc	837.48	K	Joback Method
tf	405.44	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.24	J/mol×K	653.09	Joback Method
cpg	546.08	J/mol×K	683.82	Joback Method
cpg	559.22	J/mol×K	714.55	Joback Method
cpg	571.66	J/mol×K	745.29	Joback Method
cpg	583.40	J/mol×K	776.02	Joback Method
cpg	594.46	J/mol×K	806.75	Joback Method
cpg	604.84	J/mol×K	837.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392776&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume