DL-Alanine, N-methyl-N-(3-chloro-2-methylpropoxycarbonyl)-, butyl ester

Inchi: InChI=1S/C13H24ClNO4/c1-5-6-7-18-12(16)11(3)15(4)13(17)19-9-10(2)8-14/h10-11H,5-

InchiKey: HEAIYRORUHUARO-UHFFFAOYSA-N

Formula: C13H24ClNO4

SMILES: CCCCOC(=O)C(C)N(C)C(=O)OCC(C)CCl

Mol. weight [g/mol]: 293.79

Physical Properties

Property code	Value	Unit	Source
gf	-315.29	kJ/mol	Joback Method
hf	-760.02	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.661		Crippen Method
mcvol	231.130	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
tb	698.41	K	Joback Method
tc	883.36	K	Joback Method
tf	412.98	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.05	J/mol×K	698.41	Joback Method
cpg	654.10	J/mol×K	729.24	Joback Method
cpg	668.33	J/mol×K	760.06	Joback Method
cpg	681.76	J/mol×K	790.89	Joback Method
cpg	694.39	J/mol×K	821.71	Joback Method
cpg	706.24	J/mol×K	852.54	Joback Method
cpg	717.32	J/mol×K	883.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392766&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