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

Inchi: InChI=1S/C21H40ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-26-20(24)19(3)23(4)21(25)27-
InchiKey: SGTAFXXYGUTWDM-UHFFFAOYSA-N
Formula: C21H40ClNO4
SMILES: CCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(C)CCl
Mol. weight [g/mol]: 406.00

Physical Properties

Property code	Value	Unit	Source
gf	-247.93	kJ/mol	Joback Method
hf	-925.14	kJ/mol	Joback Method
hfus	55.89	kJ/mol	Joback Method
hvap	86.30	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.782		Crippen Method
mcvol	343.850	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	881.45	K	Joback Method
tc	1079.29	K	Joback Method
tf	503.14	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.35	J/mol×K	881.45	Joback Method
cpg	1124.29	J/mol×K	914.42	Joback Method
cpg	1140.99	J/mol×K	947.40	Joback Method
cpg	1156.49	J/mol×K	980.37	Joback Method
cpg	1170.81	J/mol×K	1013.34	Joback Method
cpg	1184.00	J/mol×K	1046.32	Joback Method
cpg	1196.08	J/mol×K	1079.29	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=U392774&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume