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

Inchi: InChI=1S/C16H30ClNO4/c1-7-8-14(11(2)3)22-15(19)13(5)18(6)16(20)21-10-12(4)9-17/h

InchiKey: MGLXLEYWLSWYPS-UHFFFAOYSA-N

Formula: C16H30ClNO4

SMILES: CCCC(OC(=O)C(C)N(C)C(=O)OCC(C)CCl)C(C)C

Mol. weight [g/mol]: 335.87

Physical Properties

Property code	Value	Unit	Source
gf	-294.91	kJ/mol	Joback Method
hf	-832.50	kJ/mol	Joback Method
hfus	35.90	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.686		Crippen Method
mcvol	273.400	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	766.17	K	Joback Method
tc	954.75	K	Joback Method
tf	416.79	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.44	J/mol×K	766.17	Joback Method
cpg	824.96	J/mol×K	797.60	Joback Method
cpg	840.48	J/mol×K	829.03	Joback Method
cpg	855.03	J/mol×K	860.46	Joback Method
cpg	868.62	J/mol×K	891.89	Joback Method
cpg	881.26	J/mol×K	923.32	Joback Method
cpg	892.98	J/mol×K	954.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392768&Units=SI

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