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

Inchi: InChI=1S/C15H28ClNO4/c1-5-6-7-8-9-20-14(18)13(3)17(4)15(19)21-11-12(2)10-16/h12-
InchiKey: ZOUPGIACDVMQQM-UHFFFAOYSA-N
Formula: C15H28ClNO4
SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)OCC(C)CCl
Mol. weight [g/mol]: 321.84

Physical Properties

Property code	Value	Unit	Source
gf	-298.45	kJ/mol	Joback Method
hf	-801.30	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.442		Crippen Method
mcvol	259.310	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	744.17	K	Joback Method
tc	928.55	K	Joback Method
tf	435.52	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.23	J/mol×K	744.17	Joback Method
cpg	766.05	J/mol×K	774.90	Joback Method
cpg	780.98	J/mol×K	805.63	Joback Method
cpg	795.03	J/mol×K	836.36	Joback Method
cpg	808.21	J/mol×K	867.09	Joback Method
cpg	820.54	J/mol×K	897.82	Joback Method
cpg	832.04	J/mol×K	928.55	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=U392767&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