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

Inchi: InChI=1S/C12H22ClNO4/c1-5-6-17-11(15)10(3)14(4)12(16)18-8-9(2)7-13/h9-10H,5-8H2,

InchiKey: CYXKJWYMIOQBIG-UHFFFAOYSA-N

Formula: C12H22ClNO4

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

Mol. weight [g/mol]: 279.76

Physical Properties

Property code	Value	Unit	Source
gf	-323.71	kJ/mol	Joback Method
hf	-739.38	kJ/mol	Joback Method
hfus	32.58	kJ/mol	Joback Method
hvap	66.27	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.271		Crippen Method
mcvol	217.040	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	675.53	K	Joback Method
tc	861.48	K	Joback Method
tf	401.71	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.23	J/mol×K	675.53	Joback Method
cpg	599.83	J/mol×K	706.52	Joback Method
cpg	613.66	J/mol×K	737.51	Joback Method
cpg	626.72	J/mol×K	768.50	Joback Method
cpg	639.02	J/mol×K	799.49	Joback Method
cpg	650.56	J/mol×K	830.49	Joback Method
cpg	661.37	J/mol×K	861.48	Joback Method

Sources

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=U392765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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