DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, heptyl ester

Inchi: InChI=1S/C15H28ClNO4/c1-4-5-6-7-8-11-20-14(18)13(2)17(3)15(19)21-12-9-10-16/h13H
Inchikey: SSBVBVPJGZVGMH-UHFFFAOYSA-N
Formula: C15H28ClNO4
SMILES: CCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 321.84

Physical Properties

Property code	Value	Unit	Source
gf	-296.01	kJ/mol	Joback Method
hf	-796.02	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.586		Crippen Method
mcvol	259.310	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2094.00		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	744.61	K	Joback Method
tc	927.07	K	Joback Method
tf	450.52	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.71	J/mol×K	744.61	Joback Method
cpg	765.36	J/mol×K	775.02	Joback Method
cpg	780.14	J/mol×K	805.43	Joback Method
cpg	794.06	J/mol×K	835.84	Joback Method
cpg	807.14	J/mol×K	866.25	Joback Method
cpg	819.40	J/mol×K	896.66	Joback Method
cpg	830.84	J/mol×K	927.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392779&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