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

Inchi: InChI=1S/C19H36ClNO4/c1-4-5-6-7-8-9-10-11-12-15-24-18(22)17(2)21(3)19(23)25-16-1
InchiKey: UXVXITMDJFIHNF-UHFFFAOYSA-N
Formula: C19H36ClNO4
SMILES: CCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 377.95

Physical Properties

Property code	Value	Unit	Source
gf	-262.33	kJ/mol	Joback Method
hf	-878.58	kJ/mol	Joback Method
hfus	54.23	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.146		Crippen Method
mcvol	315.670	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	836.13	K	Joback Method
tc	1025.78	K	Joback Method
tf	495.60	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.98	J/mol×K	836.13	Joback Method
cpg	1001.12	J/mol×K	867.74	Joback Method
cpg	1017.18	J/mol×K	899.35	Joback Method
cpg	1032.19	J/mol×K	930.95	Joback Method
cpg	1046.17	J/mol×K	962.56	Joback Method
cpg	1059.15	J/mol×K	994.17	Joback Method
cpg	1071.15	J/mol×K	1025.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392783&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