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

Inchi: InChI=1S/C25H48ClNO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-30-24(28)23(2)27(3)25(29)31-22-19-20-26/h23H,4-22H2,1-3H3/t23-/m0/s1

InchiKey: LIDSLBJINJRGNI-UHFFFAOYSA-N

Formula: C25H48ClNO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl

Mol. weight [g/mol]: 462.11

Physical Properties

Property code	Value	Unit	Source
gf	-211.81	kJ/mol	Joback Method
hf	-1002.42	kJ/mol	Joback Method
hfus	69.78	kJ/mol	Joback Method
hvap	95.60	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.487		Crippen Method
mcvol	400.210	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook
tb	973.41	K	Joback Method
tc	1199.40	K	Joback Method
tf	563.22	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1356.71	J/mol×K	973.41	Joback Method
cpg	1376.67	J/mol×K	1011.08	Joback Method
cpg	1394.95	J/mol×K	1048.74	Joback Method
cpg	1411.62	J/mol×K	1086.41	Joback Method
cpg	1426.74	J/mol×K	1124.07	Joback Method
cpg	1440.37	J/mol×K	1161.74	Joback Method
cpg	1452.58	J/mol×K	1199.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392789&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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