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

Inchi: InChI=1S/C24H46ClNO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-29-23(27)22(2)26(
InchiKey: GJBINCPJPDLJQH-UHFFFAOYSA-N
Formula: C24H46ClNO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 448.08

Physical Properties

Property code	Value	Unit	Source
gf	-220.23	kJ/mol	Joback Method
hf	-981.78	kJ/mol	Joback Method
hfus	67.19	kJ/mol	Joback Method
hvap	93.37	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	7.097		Crippen Method
mcvol	386.120	ml/mol	McGowan Method
pc	834.83	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	950.53	K	Joback Method
tc	1167.79	K	Joback Method
tf	551.95	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1293.27	J/mol×K	950.53	Joback Method
cpg	1312.67	J/mol×K	986.74	Joback Method
cpg	1330.53	J/mol×K	1022.95	Joback Method
cpg	1346.90	J/mol×K	1059.16	Joback Method
cpg	1361.84	J/mol×K	1095.37	Joback Method
cpg	1375.39	J/mol×K	1131.58	Joback Method
cpg	1387.63	J/mol×K	1167.79	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=U392788&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