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

Inchi: InChI=1S/C26H50ClNO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-31-25(29)24
InchiKey: AJZUYOZMCXDMLG-UHFFFAOYSA-N
Formula: C26H50ClNO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 476.13

Physical Properties

Property code	Value	Unit	Source
gf	-203.39	kJ/mol	Joback Method
hf	-1023.06	kJ/mol	Joback Method
hfus	72.37	kJ/mol	Joback Method
hvap	97.82	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.877		Crippen Method
mcvol	414.300	ml/mol	McGowan Method
pc	749.38	kPa	Joback Method
rinpol	3172.00		NIST Webbook
rinpol	3172.00		NIST Webbook
tb	996.29	K	Joback Method
tc	1232.29	K	Joback Method
tf	574.49	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1420.55	J/mol×K	996.29	Joback Method
cpg	1441.12	J/mol×K	1035.62	Joback Method
cpg	1459.85	J/mol×K	1074.96	Joback Method
cpg	1476.82	J/mol×K	1114.29	Joback Method
cpg	1492.11	J/mol×K	1153.62	Joback Method
cpg	1505.79	J/mol×K	1192.95	Joback Method
cpg	1517.95	J/mol×K	1232.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392790&Units=SI

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