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

Inchi: InChI=1S/C16H30ClNO4/c1-4-5-6-7-8-9-12-21-15(19)14(2)18(3)16(20)22-13-10-11-17/h
InchiKey: SQSHVEUTGCRIIX-UHFFFAOYSA-N
Formula: C16H30ClNO4
SMILES: CCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 335.87

Physical Properties

Property code	Value	Unit	Source
gf	-287.59	kJ/mol	Joback Method
hf	-816.66	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.976		Crippen Method
mcvol	273.400	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	767.49	K	Joback Method
tc	950.76	K	Joback Method
tf	461.79	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.91	J/mol×K	767.49	Joback Method
cpg	822.93	J/mol×K	798.03	Joback Method
cpg	838.04	J/mol×K	828.58	Joback Method
cpg	852.25	J/mol×K	859.12	Joback Method
cpg	865.59	J/mol×K	889.67	Joback Method
cpg	878.05	J/mol×K	920.21	Joback Method
cpg	889.67	J/mol×K	950.76	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=U392780&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