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

Inchi: InChI=1S/C20H38ClNO4/c1-4-5-6-7-8-9-10-11-12-13-16-25-19(23)18(2)22(3)20(24)26-1
InchiKey: SUKRQIWGSOVGMY-UHFFFAOYSA-N
Formula: C20H38ClNO4
SMILES: CCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 391.97

Physical Properties

Property code	Value	Unit	Source
gf	-253.91	kJ/mol	Joback Method
hf	-899.22	kJ/mol	Joback Method
hfus	56.82	kJ/mol	Joback Method
hvap	84.47	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.536		Crippen Method
mcvol	329.760	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	859.01	K	Joback Method
tc	1052.30	K	Joback Method
tf	506.87	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.60	J/mol×K	859.01	Joback Method
cpg	1062.13	J/mol×K	891.23	Joback Method
cpg	1078.52	J/mol×K	923.44	Joback Method
cpg	1093.79	J/mol×K	955.66	Joback Method
cpg	1107.96	J/mol×K	987.87	Joback Method
cpg	1121.08	J/mol×K	1020.09	Joback Method
cpg	1133.16	J/mol×K	1052.30	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=U392784&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