DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(3-chloropropoxycarbonyl)-, nonyl ester

Inchi: InChI=1S/C21H39ClN2O5/c1-6-7-8-9-10-11-12-15-28-20(26)18(3)23(4)19(25)17(2)24(5)21(27)29-16-13-14-22/h17-18H,6-16H2,1-5H3

InchiKey: RITFJYUFJFEZJH-UHFFFAOYSA-N

Formula: C21H39ClN2O5

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

Mol. weight [g/mol]: 435.00

Physical Properties

Property code	Value	Unit	Source
gf	-266.07	kJ/mol	Joback Method
hf	-970.19	kJ/mol	Joback Method
hfus	60.51	kJ/mol	Joback Method
hvap	95.09	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.213		Crippen Method
mcvol	355.400	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	947.76	K	Joback Method
tc	1160.93	K	Joback Method
tf	585.54	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1168.54	J/mol×K	947.76	Joback Method
cpg	1184.96	J/mol×K	983.29	Joback Method
cpg	1199.99	J/mol×K	1018.82	Joback Method
cpg	1213.70	J/mol×K	1054.34	Joback Method
cpg	1226.12	J/mol×K	1089.87	Joback Method
cpg	1237.30	J/mol×K	1125.40	Joback Method
cpg	1247.31	J/mol×K	1160.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393236&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