DL-Valyl-DL-Valine, N,N'-dimethyl-N'-(3-chloropropoxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C21H39ClN2O5/c1-8-9-10-13-28-20(26)18(16(4)5)23(6)19(25)17(15(2)3)24(7)21(27)29-14-11-12-22/h15-18H,8-14H2,1-7H3

InchiKey: CZCWZIMDFOJTOA-UHFFFAOYSA-N

Formula: C21H39ClN2O5

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

Mol. weight [g/mol]: 435.00

Physical Properties

Property code	Value	Unit	Source
gf	-270.95	kJ/mol	Joback Method
hf	-980.75	kJ/mol	Joback Method
hfus	53.47	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.925		Crippen Method
mcvol	355.400	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	946.88	K	Joback Method
tc	1159.30	K	Joback Method
tf	555.54	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.38	J/mol×K	946.88	Joback Method
cpg	1185.66	J/mol×K	982.28	Joback Method
cpg	1200.54	J/mol×K	1017.69	Joback Method
cpg	1214.07	J/mol×K	1053.09	Joback Method
cpg	1226.31	J/mol×K	1088.49	Joback Method
cpg	1237.29	J/mol×K	1123.89	Joback Method
cpg	1247.07	J/mol×K	1159.30	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=U392991&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