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

Inchi: InChI=1S/C19H35ClN2O5/c1-6-7-8-9-10-13-26-18(24)16(3)21(4)17(23)15(2)22(5)19(25)
Inchikey: GHUSXEPLPIZGNF-UHFFFAOYSA-N
Formula: C19H35ClN2O5
SMILES: CCCCCCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 406.94

Physical Properties

Property code	Value	Unit	Source
gf	-282.91	kJ/mol	Joback Method
hf	-928.91	kJ/mol	Joback Method
hfus	55.33	kJ/mol	Joback Method
hvap	90.64	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.433		Crippen Method
mcvol	327.220	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook
tb	902.00	K	Joback Method
tc	1104.70	K	Joback Method
tf	563.00	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.78	J/mol×K	902.00	Joback Method
cpg	1062.48	J/mol×K	935.78	Joback Method
cpg	1076.97	J/mol×K	969.57	Joback Method
cpg	1090.29	J/mol×K	1003.35	Joback Method
cpg	1102.46	J/mol×K	1037.13	Joback Method
cpg	1113.54	J/mol×K	1070.92	Joback Method
cpg	1123.55	J/mol×K	1104.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393247&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