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

Inchi: InChI=1S/C19H34Cl2N2O5/c1-13(2)15(23(6)19(26)28-12-8-10-21)17(24)22(5)16(14(3)4)
InchiKey: KLMAIQZICJOYTN-UHFFFAOYSA-N
Formula: C19H34Cl2N2O5
SMILES: CC(C)C(C(=O)N(C)C(C(=O)OCCCCl)C(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 441.39

Physical Properties

Property code	Value	Unit	Source
gf	-299.72	kJ/mol	Joback Method
hf	-955.21	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	94.25	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.363		Crippen Method
mcvol	339.460	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	938.55	K	Joback Method
tc	1149.43	K	Joback Method
tf	562.92	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.72	J/mol×K	938.55	Joback Method
cpg	1088.30	J/mol×K	973.70	Joback Method
cpg	1101.59	J/mol×K	1008.84	Joback Method
cpg	1113.66	J/mol×K	1043.99	Joback Method
cpg	1124.53	J/mol×K	1079.14	Joback Method
cpg	1134.26	J/mol×K	1114.28	Joback Method
cpg	1142.89	J/mol×K	1149.43	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=U392993&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