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

Inchi: InChI=1S/C20H37ClN2O5/c1-8-9-12-27-19(25)17(15(4)5)22(6)18(24)16(14(2)3)23(7)20(

InchiKey: XTDGDRQYVOOQJL-UHFFFAOYSA-N

Formula: C20H37ClN2O5

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

Mol. weight [g/mol]: 420.97

Physical Properties

Property code	Value	Unit	Source
gf	-279.37	kJ/mol	Joback Method
hf	-960.11	kJ/mol	Joback Method
hfus	50.88	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.535		Crippen Method
mcvol	341.310	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	924.00	K	Joback Method
tc	1131.47	K	Joback Method
tf	544.27	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.28	J/mol×K	924.00	Joback Method
cpg	1124.26	J/mol×K	958.58	Joback Method
cpg	1138.93	J/mol×K	993.16	Joback Method
cpg	1152.33	J/mol×K	1027.73	Joback Method
cpg	1164.50	J/mol×K	1062.31	Joback Method
cpg	1175.48	J/mol×K	1096.89	Joback Method
cpg	1185.31	J/mol×K	1131.47	Joback Method

Sources

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=U392990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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