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

Inchi: InChI=1S/C24H45ClN2O5/c1-8-9-10-11-12-13-16-31-23(29)21(19(4)5)26(6)22(28)20(18(

InchiKey: KYVQFZZZSWLSHF-UHFFFAOYSA-N

Formula: C24H45ClN2O5

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

Mol. weight [g/mol]: 477.08

Physical Properties

Property code	Value	Unit	Source
gf	-245.69	kJ/mol	Joback Method
hf	-1042.67	kJ/mol	Joback Method
hfus	61.24	kJ/mol	Joback Method
hvap	100.99	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.095		Crippen Method
mcvol	397.670	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	2878.00		NIST Webbook
rinpol	2878.00		NIST Webbook
tb	1015.52	K	Joback Method
tc	1249.29	K	Joback Method
tf	589.35	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.45	J/mol×K	1015.52	Joback Method
cpg	1372.77	J/mol×K	1054.48	Joback Method
cpg	1388.37	J/mol×K	1093.44	Joback Method
cpg	1402.32	J/mol×K	1132.41	Joback Method
cpg	1414.71	J/mol×K	1171.37	Joback Method
cpg	1425.60	J/mol×K	1210.33	Joback Method
cpg	1435.09	J/mol×K	1249.29	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=U392992&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