DL-Valine, N-methyl-N-(3-chloropropoxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C24H46ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-19-29-23(27)22(21(2)3)26(
InchiKey: RVFNFAZWBSKMPG-UHFFFAOYSA-N
Formula: C24H46ClNO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 448.08

Physical Properties

Property code	Value	Unit	Source
gf	-222.67	kJ/mol	Joback Method
hf	-987.06	kJ/mol	Joback Method
hfus	63.66	kJ/mol	Joback Method
hvap	92.98	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.953		Crippen Method
mcvol	386.120	ml/mol	McGowan Method
pc	838.70	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	950.09	K	Joback Method
tc	1166.21	K	Joback Method
tf	536.95	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1293.65	J/mol×K	950.09	Joback Method
cpg	1312.91	J/mol×K	986.11	Joback Method
cpg	1330.63	J/mol×K	1022.13	Joback Method
cpg	1346.87	J/mol×K	1058.15	Joback Method
cpg	1361.67	J/mol×K	1094.17	Joback Method
cpg	1375.10	J/mol×K	1130.19	Joback Method
cpg	1387.20	J/mol×K	1166.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392984&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

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