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

Inchi: InChI=1S/C22H42ClNO4/c1-5-6-7-8-9-10-11-12-13-14-17-27-21(25)20(19(2)3)24(4)22(2

InchiKey: DWVUGMDHZLUWRE-UHFFFAOYSA-N

Formula: C22H42ClNO4

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

Mol. weight [g/mol]: 420.03

Physical Properties

Property code	Value	Unit	Source
gf	-239.51	kJ/mol	Joback Method
hf	-945.78	kJ/mol	Joback Method
hfus	58.48	kJ/mol	Joback Method
hvap	88.53	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.172		Crippen Method
mcvol	357.940	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	904.33	K	Joback Method
tc	1107.25	K	Joback Method
tf	514.41	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1168.25	J/mol×K	904.33	Joback Method
cpg	1186.59	J/mol×K	938.15	Joback Method
cpg	1203.61	J/mol×K	971.97	Joback Method
cpg	1219.35	J/mol×K	1005.79	Joback Method
cpg	1233.83	J/mol×K	1039.61	Joback Method
cpg	1247.11	J/mol×K	1073.43	Joback Method
cpg	1259.22	J/mol×K	1107.25	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=U392982&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