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

Inchi: InChI=1S/C27H52ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-32-26(30)25(2
InchiKey: WHKJDGXAQARRHC-UHFFFAOYSA-N
Formula: C27H52ClNO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 490.16

Physical Properties

Property code	Value	Unit	Source
gf	-197.41	kJ/mol	Joback Method
hf	-1048.98	kJ/mol	Joback Method
hfus	71.43	kJ/mol	Joback Method
hvap	99.66	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	8.123		Crippen Method
mcvol	428.390	ml/mol	McGowan Method
pc	714.54	kPa	Joback Method
rinpol	3226.00		NIST Webbook
rinpol	3226.00		NIST Webbook
tb	1018.73	K	Joback Method
tc	1263.56	K	Joback Method
tf	570.76	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1485.01	J/mol×K	1018.73	Joback Method
cpg	1505.96	J/mol×K	1059.53	Joback Method
cpg	1524.91	J/mol×K	1100.34	Joback Method
cpg	1541.94	J/mol×K	1141.14	Joback Method
cpg	1557.17	J/mol×K	1181.95	Joback Method
cpg	1570.67	J/mol×K	1222.75	Joback Method
cpg	1582.54	J/mol×K	1263.56	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=U392987&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