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

Inchi: InChI=1S/C17H32ClNO4/c1-5-6-7-8-9-12-22-16(20)15(14(2)3)19(4)17(21)23-13-10-11-1

Inchikey: NWNYWUFEVKXSFB-UHFFFAOYSA-N

Formula: C17H32ClNO4

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

Mol. weight [g/mol]: 349.89

Physical Properties

Property code	Value	Unit	Source
gf	-281.61	kJ/mol	Joback Method
hf	-842.58	kJ/mol	Joback Method
hfus	45.53	kJ/mol	Joback Method
hvap	77.40	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.222		Crippen Method
mcvol	287.490	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	789.93	K	Joback Method
tc	975.97	K	Joback Method
tf	458.06	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.58	J/mol×K	789.93	Joback Method
cpg	882.09	J/mol×K	820.94	Joback Method
cpg	897.62	J/mol×K	851.94	Joback Method
cpg	912.19	J/mol×K	882.95	Joback Method
cpg	925.81	J/mol×K	913.96	Joback Method
cpg	938.49	J/mol×K	944.97	Joback Method
cpg	950.27	J/mol×K	975.97	Joback Method

Sources

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=U392977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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