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

Inchi: InChI=1S/C19H36ClNO4/c1-5-6-7-8-9-10-11-14-24-18(22)17(16(2)3)21(4)19(23)25-15-1

InchiKey: BVUYANXWWDCTPW-UHFFFAOYSA-N

Formula: C19H36ClNO4

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

Mol. weight [g/mol]: 377.95

Physical Properties

Property code	Value	Unit	Source
gf	-264.77	kJ/mol	Joback Method
hf	-883.86	kJ/mol	Joback Method
hfus	50.71	kJ/mol	Joback Method
hvap	81.85	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	5.002		Crippen Method
mcvol	315.670	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	835.69	K	Joback Method
tc	1026.06	K	Joback Method
tf	480.60	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.47	J/mol×K	835.69	Joback Method
cpg	1001.67	J/mol×K	867.42	Joback Method
cpg	1017.78	J/mol×K	899.15	Joback Method
cpg	1032.81	J/mol×K	930.88	Joback Method
cpg	1046.80	J/mol×K	962.60	Joback Method
cpg	1059.76	J/mol×K	994.33	Joback Method
cpg	1071.73	J/mol×K	1026.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392979&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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