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

Inchi: InChI=1S/C18H34ClNO4/c1-5-6-7-8-9-10-13-23-17(21)16(15(2)3)20(4)18(22)24-14-11-1
InchiKey: CFYJHAFIYPWJSD-UHFFFAOYSA-N
Formula: C18H34ClNO4
SMILES: CCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 363.92

Physical Properties

Property code	Value	Unit	Source
gf	-273.19	kJ/mol	Joback Method
hf	-863.22	kJ/mol	Joback Method
hfus	48.12	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.612		Crippen Method
mcvol	301.580	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	812.81	K	Joback Method
tc	1000.66	K	Joback Method
tf	469.33	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.62	J/mol×K	812.81	Joback Method
cpg	941.47	J/mol×K	844.12	Joback Method
cpg	957.29	J/mol×K	875.43	Joback Method
cpg	972.09	J/mol×K	906.73	Joback Method
cpg	985.90	J/mol×K	938.04	Joback Method
cpg	998.73	J/mol×K	969.35	Joback Method
cpg	1010.62	J/mol×K	1000.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392978&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