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

Inchi: InChI=1S/C13H23Cl2NO4/c1-10(2)11(12(17)19-8-4-6-14)16(3)13(18)20-9-5-7-15/h10-11
InchiKey: IKGOABKMCRSBFU-UHFFFAOYSA-N
Formula: C13H23Cl2NO4
SMILES: CC(C)C(C(=O)OCCCCl)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 328.23

Physical Properties

Property code	Value	Unit	Source
gf	-327.22	kJ/mol	Joback Method
hf	-775.76	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.880		Crippen Method
mcvol	243.370	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	735.84	K	Joback Method
tc	925.18	K	Joback Method
tf	442.90	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.64	J/mol×K	735.84	Joback Method
cpg	681.75	J/mol×K	767.40	Joback Method
cpg	695.02	J/mol×K	798.95	Joback Method
cpg	707.46	J/mol×K	830.51	Joback Method
cpg	719.09	J/mol×K	862.07	Joback Method
cpg	729.92	J/mol×K	893.63	Joback Method
cpg	739.96	J/mol×K	925.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392989&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

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