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

Inchi: InChI=1S/C23H44ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-18-28-22(26)21(20(2)3)25(4)2
InchiKey: CXDIJAJXIQLSHL-UHFFFAOYSA-N
Formula: C23H44ClNO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 434.05

Physical Properties

Property code	Value	Unit	Source
gf	-231.09	kJ/mol	Joback Method
hf	-966.42	kJ/mol	Joback Method
hfus	61.07	kJ/mol	Joback Method
hvap	90.76	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.562		Crippen Method
mcvol	372.030	ml/mol	McGowan Method
pc	887.35	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	927.21	K	Joback Method
tc	1136.19	K	Joback Method
tf	525.68	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.70	J/mol×K	927.21	Joback Method
cpg	1249.48	J/mol×K	962.04	Joback Method
cpg	1266.84	J/mol×K	996.87	Joback Method
cpg	1282.82	J/mol×K	1031.70	Joback Method
cpg	1297.47	J/mol×K	1066.53	Joback Method
cpg	1310.83	J/mol×K	1101.36	Joback Method
cpg	1322.95	J/mol×K	1136.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392983&Units=SI

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

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