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

Inchi: InChI=1S/C25H48ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-20-30-24(28)23(22(2)3)27(4)25(29)31-21-18-19-26/h22-23H,5-21H2,1-4H3

InchiKey: DAHBXFMMHFPNES-UHFFFAOYSA-N

Formula: C25H48ClNO4

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

Mol. weight [g/mol]: 462.11

Physical Properties

Property code	Value	Unit	Source
gf	-214.25	kJ/mol	Joback Method
hf	-1007.70	kJ/mol	Joback Method
hfus	66.25	kJ/mol	Joback Method
hvap	95.21	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	7.343		Crippen Method
mcvol	400.210	ml/mol	McGowan Method
pc	793.94	kPa	Joback Method
rinpol	3006.00		NIST Webbook
rinpol	3006.00		NIST Webbook
tb	972.97	K	Joback Method
tc	1197.38	K	Joback Method
tf	548.22	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1357.05	J/mol×K	972.97	Joback Method
cpg	1376.83	J/mol×K	1010.37	Joback Method
cpg	1394.94	J/mol×K	1047.77	Joback Method
cpg	1411.44	J/mol×K	1085.18	Joback Method
cpg	1426.39	J/mol×K	1122.58	Joback Method
cpg	1439.86	J/mol×K	1159.98	Joback Method
cpg	1451.92	J/mol×K	1197.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392985&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