DL-Valine, N-methyl-N-(but-3-en-1-yloxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C25H47NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-21-29-24(27)23(22(3)4)26
InchiKey: MWYUIOCSCNSSBZ-UHFFFAOYSA-N
Formula: C25H47NO4
SMILES: C=CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
gf	-114.48	kJ/mol	Joback Method
hf	-866.53	kJ/mol	Joback Method
hfus	60.77	kJ/mol	Joback Method
hvap	90.15	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.900		Crippen Method
mcvol	383.670	ml/mol	McGowan Method
pc	830.50	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	932.22	K	Joback Method
tc	1143.64	K	Joback Method
tf	516.54	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.29	J/mol×K	932.22	Joback Method
cpg	1317.45	J/mol×K	967.46	Joback Method
cpg	1336.11	J/mol×K	1002.69	Joback Method
cpg	1353.33	J/mol×K	1037.93	Joback Method
cpg	1369.17	J/mol×K	1073.17	Joback Method
cpg	1383.68	J/mol×K	1108.40	Joback Method
cpg	1396.92	J/mol×K	1143.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392966&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