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

Inchi: InChI=1S/C27H51NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-23-31-26(29)25(24
InchiKey: KTKGQOWVVCNRLT-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: C=CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
gf	-97.64	kJ/mol	Joback Method
hf	-907.81	kJ/mol	Joback Method
hfus	65.96	kJ/mol	Joback Method
hvap	94.61	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.680		Crippen Method
mcvol	411.850	ml/mol	McGowan Method
pc	745.70	kPa	Joback Method
rinpol	2962.00		NIST Webbook
rinpol	2962.00		NIST Webbook
tb	977.98	K	Joback Method
tc	1206.47	K	Joback Method
tf	539.08	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1425.37	J/mol×K	977.98	Joback Method
cpg	1446.69	J/mol×K	1016.06	Joback Method
cpg	1466.24	J/mol×K	1054.14	Joback Method
cpg	1484.10	J/mol×K	1092.23	Joback Method
cpg	1500.36	J/mol×K	1130.31	Joback Method
cpg	1515.09	J/mol×K	1168.39	Joback Method
cpg	1528.38	J/mol×K	1206.47	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=U392968&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