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

Inchi: InChI=1S/C27H49NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-23-31-26(29)25(24
InchiKey: MZQJLNFKTXQFBJ-UHFFFAOYSA-N
Formula: C27H49NO4
SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 451.68

Physical Properties

Property code	Value	Unit	Source
gf	37.59	kJ/mol	Joback Method
hf	-741.34	kJ/mol	Joback Method
hfus	70.21	kJ/mol	Joback Method
hvap	95.13	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.127		Crippen Method
mcvol	407.550	ml/mol	McGowan Method
pc	790.82	kPa	Joback Method
rinpol	2950.00		NIST Webbook
rinpol	2950.00		NIST Webbook
tb	971.42	K	Joback Method
tc	1194.42	K	Joback Method
tf	587.81	K	Joback Method
vc	1.563	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1392.86	J/mol×K	971.42	Joback Method
cpg	1413.33	J/mol×K	1008.59	Joback Method
cpg	1432.19	J/mol×K	1045.75	Joback Method
cpg	1449.51	J/mol×K	1082.92	Joback Method
cpg	1465.37	J/mol×K	1120.08	Joback Method
cpg	1479.84	J/mol×K	1157.25	Joback Method
cpg	1492.99	J/mol×K	1194.42	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=U392942&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