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

Inchi: InChI=1S/C25H45NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-21-29-24(27)23(22(3)4)26
InchiKey: DFRNCLKESUPNPZ-UHFFFAOYSA-N
Formula: C25H45NO4
SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 423.63

Physical Properties

Property code	Value	Unit	Source
gf	20.75	kJ/mol	Joback Method
hf	-700.06	kJ/mol	Joback Method
hfus	65.03	kJ/mol	Joback Method
hvap	90.68	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.347		Crippen Method
mcvol	379.370	ml/mol	McGowan Method
pc	883.67	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	925.66	K	Joback Method
tc	1133.90	K	Joback Method
tf	565.27	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.63	J/mol×K	925.66	Joback Method
cpg	1285.07	J/mol×K	960.37	Joback Method
cpg	1303.11	J/mol×K	995.07	Joback Method
cpg	1319.82	J/mol×K	1029.78	Joback Method
cpg	1335.25	J/mol×K	1064.49	Joback Method
cpg	1349.45	J/mol×K	1099.20	Joback Method
cpg	1362.48	J/mol×K	1133.90	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=U392940&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