DL-Valine, N-methyl-N-(but-2-yn-1-yloxycarbonyl)-, dodecyl ester

Inchi: InChI=1S/C23H41NO4/c1-6-8-10-11-12-13-14-15-16-17-19-27-22(25)21(20(3)4)24(5)23(
InchiKey: CFLZOHIVMKPPMK-UHFFFAOYSA-N
Formula: C23H41NO4
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
gf	-16.36	kJ/mol	Joback Method
hf	-678.38	kJ/mol	Joback Method
hfus	60.00	kJ/mol	Joback Method
hvap	88.52	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.567		Crippen Method
mcvol	351.190	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	898.78	K	Joback Method
tc	1101.01	K	Joback Method
tf	601.86	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.33	J/mol×K	898.78	Joback Method
cpg	1165.81	J/mol×K	932.48	Joback Method
cpg	1182.99	J/mol×K	966.19	Joback Method
cpg	1198.89	J/mol×K	999.89	Joback Method
cpg	1213.56	J/mol×K	1033.60	Joback Method
cpg	1227.03	J/mol×K	1067.30	Joback Method
cpg	1239.33	J/mol×K	1101.01	Joback Method

Sources

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=U392957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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