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

Inchi: InChI=1S/C24H43NO4/c1-6-8-10-11-12-13-14-15-16-17-18-20-28-23(26)22(21(3)4)25(5)
InchiKey: GOKDBURXVVYGMT-UHFFFAOYSA-N
Formula: C24H43NO4
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
gf	-7.94	kJ/mol	Joback Method
hf	-699.02	kJ/mol	Joback Method
hfus	62.59	kJ/mol	Joback Method
hvap	90.75	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.957		Crippen Method
mcvol	365.280	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2736.00		NIST Webbook
rinpol	2736.00		NIST Webbook
tb	921.66	K	Joback Method
tc	1128.38	K	Joback Method
tf	613.13	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.77	J/mol×K	921.66	Joback Method
cpg	1228.58	J/mol×K	956.11	Joback Method
cpg	1246.00	J/mol×K	990.57	Joback Method
cpg	1262.07	J/mol×K	1025.02	Joback Method
cpg	1276.84	J/mol×K	1059.48	Joback Method
cpg	1290.33	J/mol×K	1093.93	Joback Method
cpg	1302.60	J/mol×K	1128.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392958&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