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

Inchi: InChI=1S/C22H39NO4/c1-6-8-10-11-12-13-14-15-16-18-26-21(24)20(19(3)4)23(5)22(25)
InchiKey: MVPOXZYPAHETRO-UHFFFAOYSA-N
Formula: C22H39NO4
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 381.55

Physical Properties

Property code	Value	Unit	Source
gf	-24.78	kJ/mol	Joback Method
hf	-657.74	kJ/mol	Joback Method
hfus	57.41	kJ/mol	Joback Method
hvap	86.30	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.177		Crippen Method
mcvol	337.100	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook
tb	875.90	K	Joback Method
tc	1074.54	K	Joback Method
tf	590.59	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.46	J/mol×K	875.90	Joback Method
cpg	1103.64	J/mol×K	909.01	Joback Method
cpg	1120.59	J/mol×K	942.11	Joback Method
cpg	1136.34	J/mol×K	975.22	Joback Method
cpg	1150.91	J/mol×K	1008.32	Joback Method
cpg	1164.33	J/mol×K	1041.43	Joback Method
cpg	1176.64	J/mol×K	1074.54	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=U392956&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

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