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

Inchi: InChI=1S/C18H31NO4/c1-6-8-10-11-12-14-22-17(20)16(15(3)4)19(5)18(21)23-13-9-7-2/h
Inchikey: YPWXYBVHZPVIFO-UHFFFAOYSA-N
Formula: C18H31NO4
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCC)C(C)C
Mol. weight [g/mol]: 325.44

Physical Properties

Property code	Value	Unit	Source
gf	-58.46	kJ/mol	Joback Method
hf	-575.18	kJ/mol	Joback Method
hfus	47.05	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.616		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	784.38	K	Joback Method
tc	976.50	K	Joback Method
tf	545.51	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.00	J/mol×K	784.38	Joback Method
cpg	862.11	J/mol×K	816.40	Joback Method
cpg	878.20	J/mol×K	848.42	Joback Method
cpg	893.29	J/mol×K	880.44	Joback Method
cpg	907.38	J/mol×K	912.46	Joback Method
cpg	920.50	J/mol×K	944.48	Joback Method
cpg	932.66	J/mol×K	976.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392952&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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