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

Inchi: InChI=1S/C19H33NO4/c1-6-8-10-11-12-13-15-23-18(21)17(16(3)4)20(5)19(22)24-14-9-7
InchiKey: NIGAWKNZTLJVER-UHFFFAOYSA-N
Formula: C19H33NO4
SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCC)C(C)C
Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
gf	-29.77	kJ/mol	Joback Method
hf	-576.22	kJ/mol	Joback Method
hfus	49.49	kJ/mol	Joback Method
hvap	77.33	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.006		Crippen Method
mcvol	294.830	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	788.38	K	Joback Method
tc	975.30	K	Joback Method
tf	497.65	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.04	J/mol×K	788.38	Joback Method
cpg	915.25	J/mol×K	819.53	Joback Method
cpg	931.46	J/mol×K	850.69	Joback Method
cpg	946.68	J/mol×K	881.84	Joback Method
cpg	960.96	J/mol×K	913.00	Joback Method
cpg	974.31	J/mol×K	944.15	Joback Method
cpg	986.77	J/mol×K	975.30	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=U392934&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