DL-Valine, N-methyl-N-(but-2-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: LNQBFLFLZMCGRW-UHFFFAOYSA-N

Formula: C19H33NO4

SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCC)C(C)C

Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
gf	-50.04	kJ/mol	Joback Method
hf	-595.82	kJ/mol	Joback Method
hfus	49.64	kJ/mol	Joback Method
hvap	79.62	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.006		Crippen Method
mcvol	294.830	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	807.26	K	Joback Method
tc	999.95	K	Joback Method
tf	556.78	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.92	J/mol×K	807.26	Joback Method
cpg	921.30	J/mol×K	839.38	Joback Method
cpg	937.61	J/mol×K	871.49	Joback Method
cpg	952.87	J/mol×K	903.61	Joback Method
cpg	967.11	J/mol×K	935.72	Joback Method
cpg	980.33	J/mol×K	967.84	Joback Method
cpg	992.56	J/mol×K	999.95	Joback Method

Sources

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=U392953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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