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

Inchi: InChI=1S/C29H53NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-33-28(31
InchiKey: KIIKPNIXTMAUQT-UHFFFAOYSA-N
Formula: C29H53NO4
SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 479.74

Physical Properties

Property code	Value	Unit	Source
gf	54.43	kJ/mol	Joback Method
hf	-782.62	kJ/mol	Joback Method
hfus	75.39	kJ/mol	Joback Method
hvap	99.59	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	7.907		Crippen Method
mcvol	435.730	ml/mol	McGowan Method
pc	711.87	kPa	Joback Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook
tb	1017.18	K	Joback Method
tc	1259.83	K	Joback Method
tf	610.35	K	Joback Method
vc	1.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.76	J/mol×K	1017.18	Joback Method
cpg	1543.47	J/mol×K	1057.62	Joback Method
cpg	1563.29	J/mol×K	1098.06	Joback Method
cpg	1581.31	J/mol×K	1138.50	Joback Method
cpg	1597.63	J/mol×K	1178.94	Joback Method
cpg	1612.37	J/mol×K	1219.38	Joback Method
cpg	1625.61	J/mol×K	1259.83	Joback Method

Sources

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=U392944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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