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

Inchi: InChI=1S/C28H51NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-24-32-27(30)26
Inchikey: AHWNKMWQJKRQOU-UHFFFAOYSA-N
Formula: C28H51NO4
SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 465.71

Physical Properties

Property code	Value	Unit	Source
gf	46.01	kJ/mol	Joback Method
hf	-761.98	kJ/mol	Joback Method
hfus	72.80	kJ/mol	Joback Method
hvap	97.36	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	7.517		Crippen Method
mcvol	421.640	ml/mol	McGowan Method
pc	749.79	kPa	Joback Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		NIST Webbook
tb	994.30	K	Joback Method
tc	1226.46	K	Joback Method
tf	599.08	K	Joback Method
vc	1.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.12	J/mol×K	994.30	Joback Method
cpg	1478.19	J/mol×K	1032.99	Joback Method
cpg	1497.51	J/mol×K	1071.69	Joback Method
cpg	1515.17	J/mol×K	1110.38	Joback Method
cpg	1531.25	J/mol×K	1149.07	Joback Method
cpg	1545.86	J/mol×K	1187.77	Joback Method
cpg	1559.06	J/mol×K	1226.46	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=U392943&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