DL-Alanine, N-methyl-N-(byt-2-yn-1-yloxycarbonyl)-, octadecyl ester

Inchi: InChI=1S/C27H49NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-31-26(29)2
InchiKey: PHPKFRJDFLFVDY-UHFFFAOYSA-N
Formula: C27H49NO4
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 451.68

Physical Properties

Property code	Value	Unit	Source
gf	19.76	kJ/mol	Joback Method
hf	-755.66	kJ/mol	Joback Method
hfus	73.88	kJ/mol	Joback Method
hvap	97.81	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.271		Crippen Method
mcvol	407.550	ml/mol	McGowan Method
pc	792.60	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	990.74	K	Joback Method
tc	1218.49	K	Joback Method
tf	661.94	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.69	J/mol×K	990.74	Joback Method
cpg	1419.85	J/mol×K	1028.70	Joback Method
cpg	1438.28	J/mol×K	1066.66	Joback Method
cpg	1455.06	J/mol×K	1104.62	Joback Method
cpg	1470.25	J/mol×K	1142.58	Joback Method
cpg	1483.92	J/mol×K	1180.54	Joback Method
cpg	1496.12	J/mol×K	1218.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392729&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