DL-Alanine, N-methyl-N-(byt-3-yn-1-yloxycarbonyl)-, pentadecyl ester

Inchi: InChI=1S/C24H43NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-21-28-23(26)22(3)25(4)24(27)29-20-8-6-2/h22H,5,7,9-21H2,1-4H3/t22-/m0/s1

InchiKey: DBTGMITXJGIYSC-UHFFFAOYSA-N

Formula: C24H43NO4

SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
gf	14.77	kJ/mol	Joback Method
hf	-674.14	kJ/mol	Joback Method
hfus	65.96	kJ/mol	Joback Method
hvap	88.84	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.101		Crippen Method
mcvol	365.280	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook
tb	903.22	K	Joback Method
tc	1105.92	K	Joback Method
tf	569.00	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.32	J/mol×K	903.22	Joback Method
cpg	1221.36	J/mol×K	937.00	Joback Method
cpg	1239.10	J/mol×K	970.79	Joback Method
cpg	1255.60	J/mol×K	1004.57	Joback Method
cpg	1270.89	J/mol×K	1038.36	Joback Method
cpg	1285.04	J/mol×K	1072.14	Joback Method
cpg	1298.08	J/mol×K	1105.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392712&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

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