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

Inchi: InChI=1S/C23H41NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-20-27-22(25)21(3)24(4)23(
InchiKey: NELPLQOASRVQMT-UHFFFAOYSA-N
Formula: C23H41NO4
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
gf	-13.92	kJ/mol	Joback Method
hf	-673.10	kJ/mol	Joback Method
hfus	63.52	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.711		Crippen Method
mcvol	351.190	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	899.22	K	Joback Method
tc	1101.18	K	Joback Method
tf	616.86	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.89	J/mol×K	899.22	Joback Method
cpg	1165.37	J/mol×K	932.88	Joback Method
cpg	1182.56	J/mol×K	966.54	Joback Method
cpg	1198.50	J/mol×K	1000.20	Joback Method
cpg	1213.21	J/mol×K	1033.86	Joback Method
cpg	1226.73	J/mol×K	1067.52	Joback Method
cpg	1239.10	J/mol×K	1101.18	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=U392726&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