DL-Alanine, N-methyl-N-(byt-3-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: HBQGZGIEFZOUJG-UHFFFAOYSA-N
Formula: C23H41NO4
SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
gf	6.35	kJ/mol	Joback Method
hf	-653.50	kJ/mol	Joback Method
hfus	63.37	kJ/mol	Joback Method
hvap	86.62	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.711		Crippen Method
mcvol	351.190	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
tb	880.34	K	Joback Method
tc	1077.89	K	Joback Method
tf	557.73	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.99	J/mol×K	880.34	Joback Method
cpg	1158.58	J/mol×K	913.27	Joback Method
cpg	1175.95	J/mol×K	946.19	Joback Method
cpg	1192.16	J/mol×K	979.12	Joback Method
cpg	1207.23	J/mol×K	1012.04	Joback Method
cpg	1221.21	J/mol×K	1044.97	Joback Method
cpg	1234.15	J/mol×K	1077.89	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=U392711&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