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

Inchi: InChI=1S/C14H23NO4/c1-5-7-9-11-18-13(16)12(3)15(4)14(17)19-10-8-6-2/h2,12H,5,7-11

InchiKey: LBRLUQCUOMSEJL-UHFFFAOYSA-N

Formula: C14H23NO4

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

Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
gf	-69.43	kJ/mol	Joback Method
hf	-467.74	kJ/mol	Joback Method
hfus	40.06	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.200		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	674.42	K	Joback Method
tc	859.47	K	Joback Method
tf	456.30	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.11	J/mol×K	674.42	Joback Method
cpg	630.28	J/mol×K	705.26	Joback Method
cpg	644.65	J/mol×K	736.10	Joback Method
cpg	658.26	J/mol×K	766.94	Joback Method
cpg	671.10	J/mol×K	797.79	Joback Method
cpg	683.20	J/mol×K	828.63	Joback Method
cpg	694.57	J/mol×K	859.47	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=U392702&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