DL-Alanine, N-methyl-N-(byt-2-yn-1-yloxycarbonyl)-, 2-methylhex-3-yl ester

Inchi: InChI=1S/C16H27NO4/c1-7-9-11-20-16(19)17(6)13(5)15(18)21-14(10-8-2)12(3)4/h12-14
InchiKey: RIIMPLQMBBFMSY-UHFFFAOYSA-N
Formula: C16H27NO4
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OC(CCC)C(C)C
Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
gf	-77.74	kJ/mol	Joback Method
hf	-539.18	kJ/mol	Joback Method
hfus	38.34	kJ/mol	Joback Method
hvap	72.55	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.834		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
tb	738.18	K	Joback Method
tc	933.55	K	Joback Method
tf	507.97	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.47	J/mol×K	738.18	Joback Method
cpg	747.25	J/mol×K	770.74	Joback Method
cpg	763.05	J/mol×K	803.30	Joback Method
cpg	777.87	J/mol×K	835.86	Joback Method
cpg	791.75	J/mol×K	868.43	Joback Method
cpg	804.67	J/mol×K	900.99	Joback Method
cpg	816.68	J/mol×K	933.55	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=U392718&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