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

InchI: InChI=1S/C22H39NO4/c1-5-7-9-10-11-12-13-14-15-16-17-19-26-21(24)20(3)23(4)22(25)
InchiKey: TZBNODJZOIFGFD-UHFFFAOYSA-N
Formula: C22H39NO4
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 381.55

Physical Properties

Property code	Value	Unit	Source
gf	-22.34	kJ/mol	Joback Method
hf	-652.46	kJ/mol	Joback Method
hfus	60.93	kJ/mol	Joback Method
hvap	86.69	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.321		Crippen Method
mcvol	337.100	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	876.34	K	Joback Method
tc	1074.36	K	Joback Method
tf	605.59	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.00	J/mol×K	876.34	Joback Method
cpg	1103.14	J/mol×K	909.34	Joback Method
cpg	1120.07	J/mol×K	942.35	Joback Method
cpg	1135.81	J/mol×K	975.35	Joback Method
cpg	1150.40	J/mol×K	1008.35	Joback Method
cpg	1163.85	J/mol×K	1041.36	Joback Method
cpg	1176.22	J/mol×K	1074.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392725&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

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