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

Inchi: InChI=1S/C19H33NO4/c1-5-7-9-10-11-12-13-14-16-23-18(21)17(3)20(4)19(22)24-15-8-6

InchiKey: LNWDBHJJAVKANV-UHFFFAOYSA-N

Formula: C19H33NO4

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

Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
gf	-27.33	kJ/mol	Joback Method
hf	-570.94	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	77.71	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.151		Crippen Method
mcvol	294.830	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	788.82	K	Joback Method
tc	974.29	K	Joback Method
tf	512.65	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.54	J/mol×K	788.82	Joback Method
cpg	914.61	J/mol×K	819.73	Joback Method
cpg	930.70	J/mol×K	850.64	Joback Method
cpg	945.84	J/mol×K	881.56	Joback Method
cpg	960.05	J/mol×K	912.47	Joback Method
cpg	973.36	J/mol×K	943.38	Joback Method
cpg	985.79	J/mol×K	974.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392707&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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