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

Inchi: InChI=1S/C20H35NO4/c1-5-7-9-10-11-12-13-14-15-17-24-19(22)18(3)21(4)20(23)25-16-
InchiKey: AYMSHITUCNYNNS-UHFFFAOYSA-N
Formula: C20H35NO4
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 353.50

Physical Properties

Property code	Value	Unit	Source
gf	-39.18	kJ/mol	Joback Method
hf	-611.18	kJ/mol	Joback Method
hfus	55.75	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.541		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	830.58	K	Joback Method
tc	1023.23	K	Joback Method
tf	583.05	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.20	J/mol×K	830.58	Joback Method
cpg	980.73	J/mol×K	862.69	Joback Method
cpg	997.16	J/mol×K	894.80	Joback Method
cpg	1012.53	J/mol×K	926.91	Joback Method
cpg	1026.84	J/mol×K	959.01	Joback Method
cpg	1040.13	J/mol×K	991.12	Joback Method
cpg	1052.42	J/mol×K	1023.23	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=U392723&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