DL-Alanine, N-methyl-N-(byt-3-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: OBQPGZOKHKVRMV-UHFFFAOYSA-N
Formula: C20H35NO4
SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 353.50

Physical Properties

Property code	Value	Unit	Source
gf	-18.91	kJ/mol	Joback Method
hf	-591.58	kJ/mol	Joback Method
hfus	55.60	kJ/mol	Joback Method
hvap	79.94	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.541		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook
tb	811.70	K	Joback Method
tc	999.04	K	Joback Method
tf	523.92	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.00	J/mol×K	811.70	Joback Method
cpg	974.42	J/mol×K	842.92	Joback Method
cpg	990.81	J/mol×K	874.15	Joback Method
cpg	1006.21	J/mol×K	905.37	Joback Method
cpg	1020.64	J/mol×K	936.60	Joback Method
cpg	1034.13	J/mol×K	967.82	Joback Method
cpg	1046.70	J/mol×K	999.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392708&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