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

Inchi: InChI=1S/C26H47NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-30-25(28)24(3
InchiKey: QPLILBUIANMJOP-UHFFFAOYSA-N
Formula: C26H47NO4
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 437.66

Physical Properties

Property code	Value	Unit	Source
gf	11.34	kJ/mol	Joback Method
hf	-735.02	kJ/mol	Joback Method
hfus	71.29	kJ/mol	Joback Method
hvap	95.59	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.881		Crippen Method
mcvol	393.460	ml/mol	McGowan Method
pc	837.24	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	967.86	K	Joback Method
tc	1187.51	K	Joback Method
tf	650.67	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.81	J/mol×K	967.86	Joback Method
cpg	1355.49	J/mol×K	1004.47	Joback Method
cpg	1373.58	J/mol×K	1041.08	Joback Method
cpg	1390.14	J/mol×K	1077.68	Joback Method
cpg	1405.22	J/mol×K	1114.29	Joback Method
cpg	1418.87	J/mol×K	1150.90	Joback Method
cpg	1431.15	J/mol×K	1187.51	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=U392728&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