DL-Alanine, N-methyl-N-(byt-4-en-1-yloxycarbonyl)-, heptadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-30-25(28)24(3
InchiKey: ZLBRHHFDVFROEI-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
gf	-103.62	kJ/mol	Joback Method
hf	-881.89	kJ/mol	Joback Method
hfus	66.89	kJ/mol	Joback Method
hvap	92.77	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.434		Crippen Method
mcvol	397.760	ml/mol	McGowan Method
pc	782.87	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	955.54	K	Joback Method
tc	1176.33	K	Joback Method
tf	542.81	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1360.76	J/mol×K	955.54	Joback Method
cpg	1381.65	J/mol×K	992.34	Joback Method
cpg	1400.90	J/mol×K	1029.14	Joback Method
cpg	1418.60	J/mol×K	1065.94	Joback Method
cpg	1434.81	J/mol×K	1102.74	Joback Method
cpg	1449.58	J/mol×K	1139.53	Joback Method
cpg	1463.01	J/mol×K	1176.33	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=U392742&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