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

Inchi: InChI=1S/C25H47NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-22-29-24(27)23(3)26
InchiKey: RURNLLFXGUIEKH-UHFFFAOYSA-N
Formula: C25H47NO4
SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
gf	-112.04	kJ/mol	Joback Method
hf	-861.25	kJ/mol	Joback Method
hfus	64.30	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.044		Crippen Method
mcvol	383.670	ml/mol	McGowan Method
pc	826.69	kPa	Joback Method
rinpol	2785.00		NIST Webbook
rinpol	2785.00		NIST Webbook
tb	932.66	K	Joback Method
tc	1145.09	K	Joback Method
tf	531.54	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.90	J/mol×K	932.66	Joback Method
cpg	1317.19	J/mol×K	968.07	Joback Method
cpg	1335.97	J/mol×K	1003.47	Joback Method
cpg	1353.32	J/mol×K	1038.88	Joback Method
cpg	1369.28	J/mol×K	1074.28	Joback Method
cpg	1383.92	J/mol×K	1109.69	Joback Method
cpg	1397.29	J/mol×K	1145.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392741&Units=SI

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