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

Inchi: InChI=1S/C27H51NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-31-26(29)2

InchiKey: DEIWRKYKURVHGT-UHFFFAOYSA-N

Formula: C27H51NO4

SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
gf	-95.20	kJ/mol	Joback Method
hf	-902.53	kJ/mol	Joback Method
hfus	69.48	kJ/mol	Joback Method
hvap	94.99	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.824		Crippen Method
mcvol	411.850	ml/mol	McGowan Method
pc	742.45	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	978.42	K	Joback Method
tc	1208.81	K	Joback Method
tf	554.08	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1425.05	J/mol×K	978.42	Joback Method
cpg	1446.59	J/mol×K	1016.82	Joback Method
cpg	1466.35	J/mol×K	1055.22	Joback Method
cpg	1484.41	J/mol×K	1093.61	Joback Method
cpg	1500.86	J/mol×K	1132.01	Joback Method
cpg	1515.77	J/mol×K	1170.41	Joback Method
cpg	1529.23	J/mol×K	1208.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392743&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

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

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