DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(byt-4-en-1-yloxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C27H50N2O5/c1-7-9-11-12-13-14-15-16-17-18-19-20-22-33-26(31)24(4)28(5)2
InchiKey: LTSUKSXIFLSHBE-UHFFFAOYSA-N
Formula: C27H50N2O5
SMILES: C=CCCOC(=O)N(C)C(C)C(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 482.70

Physical Properties

Property code	Value	Unit	Source
gf	-115.78	kJ/mol	Joback Method
hf	-952.86	kJ/mol	Joback Method
hfus	70.57	kJ/mol	Joback Method
hvap	103.39	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.111		Crippen Method
mcvol	423.400	ml/mol	McGowan Method
pc	771.18	kPa	Joback Method
rinpol	3076.00		NIST Webbook
tb	1044.29	K	Joback Method
tc	1297.69	K	Joback Method
tf	621.48	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1488.07	J/mol×K	1044.29	Joback Method
cpg	1507.94	J/mol×K	1086.52	Joback Method
cpg	1525.82	J/mol×K	1128.76	Joback Method
cpg	1541.82	J/mol×K	1170.99	Joback Method
cpg	1556.06	J/mol×K	1213.23	Joback Method
cpg	1568.67	J/mol×K	1255.46	Joback Method
cpg	1579.77	J/mol×K	1297.69	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=U392749&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