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

Inchi: InChI=1S/C19H35NO4/c1-5-7-9-10-11-12-13-14-16-23-18(21)17(3)20(4)19(22)24-15-8-6

InchiKey: BWSCUVNNJOEXOL-UHFFFAOYSA-N

Formula: C19H35NO4

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

Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
gf	-162.56	kJ/mol	Joback Method
hf	-737.41	kJ/mol	Joback Method
hfus	48.76	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.703		Crippen Method
mcvol	299.130	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	795.38	K	Joback Method
tc	978.86	K	Joback Method
tf	463.92	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.70	J/mol×K	795.38	Joback Method
cpg	943.24	J/mol×K	825.96	Joback Method
cpg	959.78	J/mol×K	856.54	Joback Method
cpg	975.34	J/mol×K	887.12	Joback Method
cpg	989.94	J/mol×K	917.70	Joback Method
cpg	1003.60	J/mol×K	948.28	Joback Method
cpg	1016.35	J/mol×K	978.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392735&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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