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

Inchi: InChI=1S/C18H33NO4/c1-5-7-9-10-11-12-13-15-22-17(20)16(3)19(4)18(21)23-14-8-6-2/l
InchiKey: MFRCOCCXGVQILP-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
gf	-170.98	kJ/mol	Joback Method
hf	-716.77	kJ/mol	Joback Method
hfus	46.17	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.313		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	772.50	K	Joback Method
tc	954.02	K	Joback Method
tf	452.65	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.39	J/mol×K	772.50	Joback Method
cpg	883.57	J/mol×K	802.75	Joback Method
cpg	899.79	J/mol×K	833.01	Joback Method
cpg	915.07	J/mol×K	863.26	Joback Method
cpg	929.44	J/mol×K	893.51	Joback Method
cpg	942.91	J/mol×K	923.76	Joback Method
cpg	955.52	J/mol×K	954.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392734&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

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