DL-Alanine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C21H39NO4/c1-7-8-9-10-13-25-20(23)17(5)22(6)21(24)26-19-14-16(4)11-12-1
InchiKey: RQSSIDYAYGIOFB-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
gf	-226.97	kJ/mol	Joback Method
hf	-895.76	kJ/mol	Joback Method
hfus	45.67	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.028		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	2265.00		NIST Webbook
rinpol	2265.00		NIST Webbook
tb	854.23	K	Joback Method
tc	1053.56	K	Joback Method
tf	472.12	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.07	J/mol×K	854.23	Joback Method
cpg	1098.95	J/mol×K	887.45	Joback Method
cpg	1117.33	J/mol×K	920.67	Joback Method
cpg	1134.23	J/mol×K	953.90	Joback Method
cpg	1149.68	J/mol×K	987.12	Joback Method
cpg	1163.68	J/mol×K	1020.34	Joback Method
cpg	1176.27	J/mol×K	1053.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392794&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