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

Inchi: InChI=1S/C22H41NO4/c1-7-8-9-10-11-14-26-21(24)18(5)23(6)22(25)27-20-15-17(4)12-1
Inchikey: ZYJKVKNGJCTJAZ-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: CCCCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
gf	-218.55	kJ/mol	Joback Method
hf	-916.40	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	83.96	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.418		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
tb	877.11	K	Joback Method
tc	1078.36	K	Joback Method
tf	483.39	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.52	J/mol×K	877.11	Joback Method
cpg	1161.42	J/mol×K	910.65	Joback Method
cpg	1179.76	J/mol×K	944.19	Joback Method
cpg	1196.55	J/mol×K	977.74	Joback Method
cpg	1211.84	J/mol×K	1011.28	Joback Method
cpg	1225.63	J/mol×K	1044.82	Joback Method
cpg	1237.96	J/mol×K	1078.36	Joback Method

Sources

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=U392795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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