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

Inchi: InChI=1S/C20H37NO4/c1-7-8-9-12-24-19(22)16(5)21(6)20(23)25-18-13-15(4)10-11-17(1

InchiKey: YMDSXADJKNPYJR-UHFFFAOYSA-N

Formula: C20H37NO4

SMILES: CCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
gf	-235.39	kJ/mol	Joback Method
hf	-875.12	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	79.50	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.638		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook
tb	831.35	K	Joback Method
tc	1029.52	K	Joback Method
tf	460.85	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.19	J/mol×K	831.35	Joback Method
cpg	1037.06	J/mol×K	864.38	Joback Method
cpg	1055.48	J/mol×K	897.41	Joback Method
cpg	1072.48	J/mol×K	930.43	Joback Method
cpg	1088.06	J/mol×K	963.46	Joback Method
cpg	1102.26	J/mol×K	996.49	Joback Method
cpg	1115.08	J/mol×K	1029.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392793&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