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

Inchi: InChI=1S/C19H35NO4/c1-12(2)11-23-18(21)15(6)20(7)19(22)24-17-10-14(5)8-9-16(17)1
InchiKey: GHSGASZEMMLCHA-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CC(C)COC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
gf	-246.25	kJ/mol	Joback Method
hf	-859.76	kJ/mol	Joback Method
hfus	36.97	kJ/mol	Joback Method
hvap	76.89	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.103		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
tb	808.03	K	Joback Method
tc	1007.80	K	Joback Method
tf	434.58	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.41	J/mol×K	808.03	Joback Method
cpg	976.48	J/mol×K	841.33	Joback Method
cpg	995.11	J/mol×K	874.62	Joback Method
cpg	1012.32	J/mol×K	907.92	Joback Method
cpg	1028.12	J/mol×K	941.21	Joback Method
cpg	1042.53	J/mol×K	974.51	Joback Method
cpg	1055.56	J/mol×K	1007.80	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=U392792&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