L-Leucine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, butyl ester

Inchi: InChI=1S/C22H41NO4/c1-8-9-12-26-21(24)19(13-15(2)3)23(7)22(25)27-20-14-17(6)10-1

InchiKey: QCTCFLPEINRDCV-UHFFFAOYSA-N

Formula: C22H41NO4

SMILES: CCCCOC(=O)C(CC(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	-220.99	kJ/mol	Joback Method
hf	-921.68	kJ/mol	Joback Method
hfus	44.74	kJ/mol	Joback Method
hvap	83.57	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.274		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook
tb	876.67	K	Joback Method
tc	1079.03	K	Joback Method
tf	468.39	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.96	J/mol×K	876.67	Joback Method
cpg	1161.95	J/mol×K	910.40	Joback Method
cpg	1180.35	J/mol×K	944.12	Joback Method
cpg	1197.19	J/mol×K	977.85	Joback Method
cpg	1212.48	J/mol×K	1011.57	Joback Method
cpg	1226.26	J/mol×K	1045.30	Joback Method
cpg	1238.55	J/mol×K	1079.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392411&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