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

Inchi: InChI=1S/C22H41NO4/c1-14(2)11-19(21(24)26-13-15(3)4)23(8)22(25)27-20-12-17(7)9-1

InchiKey: ZREMMJAEGFRXRL-UHFFFAOYSA-N

Formula: C22H41NO4

SMILES: CC(C)COC(=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	-223.43	kJ/mol	Joback Method
hf	-926.96	kJ/mol	Joback Method
hfus	41.22	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	5.130		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2233.00		NIST Webbook
rinpol	2233.00		NIST Webbook
tb	876.23	K	Joback Method
tc	1079.84	K	Joback Method
tf	453.39	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.40	J/mol×K	876.23	Joback Method
cpg	1162.50	J/mol×K	910.16	Joback Method
cpg	1180.98	J/mol×K	944.10	Joback Method
cpg	1197.85	J/mol×K	978.03	Joback Method
cpg	1213.16	J/mol×K	1011.97	Joback Method
cpg	1226.93	J/mol×K	1045.90	Joback Method
cpg	1239.17	J/mol×K	1079.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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