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

Inchi: InChI=1S/C21H39NO4/c1-8-11-25-20(23)18(12-14(2)3)22(7)21(24)26-19-13-16(6)9-10-1
InchiKey: MMYCCPWRFSFDGJ-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: CCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
gf	-229.41	kJ/mol	Joback Method
hf	-901.04	kJ/mol	Joback Method
hfus	42.15	kJ/mol	Joback Method
hvap	81.34	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.884		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	853.79	K	Joback Method
tc	1054.56	K	Joback Method
tf	457.12	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.53	J/mol×K	853.79	Joback Method
cpg	1099.54	J/mol×K	887.25	Joback Method
cpg	1118.02	J/mol×K	920.71	Joback Method
cpg	1134.99	J/mol×K	954.18	Joback Method
cpg	1150.47	J/mol×K	987.64	Joback Method
cpg	1164.48	J/mol×K	1021.10	Joback Method
cpg	1177.05	J/mol×K	1054.56	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=U392410&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