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

Inchi: InChI=1S/C27H51NO4/c1-8-9-10-11-12-13-14-17-31-26(29)24(18-20(2)3)28(7)27(30)32-
InchiKey: CWBDQVQQTFHMFV-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: CCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
gf	-178.89	kJ/mol	Joback Method
hf	-1024.88	kJ/mol	Joback Method
hfus	57.69	kJ/mol	Joback Method
hvap	94.70	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	7.224		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	991.07	K	Joback Method
tc	1214.56	K	Joback Method
tf	524.74	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1460.33	J/mol×K	991.07	Joback Method
cpg	1480.49	J/mol×K	1028.32	Joback Method
cpg	1498.57	J/mol×K	1065.57	Joback Method
cpg	1514.62	J/mol×K	1102.82	Joback Method
cpg	1528.70	J/mol×K	1140.07	Joback Method
cpg	1540.86	J/mol×K	1177.31	Joback Method
cpg	1551.16	J/mol×K	1214.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392416&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