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

Inchi: InChI=1S/C23H43NO4/c1-8-9-10-13-27-22(25)20(14-16(2)3)24(7)23(26)28-21-15-18(6)11-12-19(21)17(4)5

InchiKey: JNLSXTWDVXEFGW-UHFFFAOYSA-N

Formula: C23H43NO4

SMILES: CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
gf	-212.57	kJ/mol	Joback Method
hf	-942.32	kJ/mol	Joback Method
hfus	47.33	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.664		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	993.25	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	899.55	K	Joback Method
tc	1104.29	K	Joback Method
tf	479.66	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.89	J/mol×K	899.55	Joback Method
cpg	1224.88	J/mol×K	933.67	Joback Method
cpg	1243.20	J/mol×K	967.80	Joback Method
cpg	1259.89	J/mol×K	1001.92	Joback Method
cpg	1274.98	J/mol×K	1036.04	Joback Method
cpg	1288.50	J/mol×K	1070.17	Joback Method
cpg	1300.47	J/mol×K	1104.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392412&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