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

Inchi: InChI=1S/C24H45NO4/c1-16(2)10-9-13-28-23(26)21(14-17(3)4)25(8)24(27)29-22-15-19(

InchiKey: HFEAFMSQYQSXKI-UHFFFAOYSA-N

Formula: C24H45NO4

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

Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
gf	-206.59	kJ/mol	Joback Method
hf	-968.24	kJ/mol	Joback Method
hfus	46.40	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.910		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	921.99	K	Joback Method
tc	1130.51	K	Joback Method
tf	475.93	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.65	J/mol×K	921.99	Joback Method
cpg	1288.67	J/mol×K	956.74	Joback Method
cpg	1306.92	J/mol×K	991.50	Joback Method
cpg	1323.45	J/mol×K	1026.25	Joback Method
cpg	1338.28	J/mol×K	1061.00	Joback Method
cpg	1351.45	J/mol×K	1095.76	Joback Method
cpg	1363.00	J/mol×K	1130.51	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=U392426&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