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

Inchi: InChI=1S/C29H55NO4/c1-8-9-10-11-12-13-14-15-16-19-33-28(31)26(20-22(2)3)30(7)29(
InchiKey: ADQOYZIXKZISNF-UHFFFAOYSA-N
Formula: C29H55NO4
SMILES: CCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 481.75

Physical Properties

Property code	Value	Unit	Source
gf	-162.05	kJ/mol	Joback Method
hf	-1066.16	kJ/mol	Joback Method
hfus	62.87	kJ/mol	Joback Method
hvap	99.15	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	8.004		Crippen Method
mcvol	433.470	ml/mol	McGowan Method
pc	711.49	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	1036.83	K	Joback Method
tc	1276.26	K	Joback Method
tf	547.28	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1589.55	J/mol×K	1036.83	Joback Method
cpg	1609.92	J/mol×K	1076.73	Joback Method
cpg	1627.89	J/mol×K	1116.64	Joback Method
cpg	1643.53	J/mol×K	1156.54	Joback Method
cpg	1656.91	J/mol×K	1196.45	Joback Method
cpg	1668.10	J/mol×K	1236.35	Joback Method
cpg	1677.18	J/mol×K	1276.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392418&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