

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

InChI: InChI=1S/C24H45NO4/c1-8-9-10-11-14-28-23(26)21(15-17(2)3)25(7)24(27)29-22-16-19
InChIKey: ILZZALLKXXWHIA-UHFFFAOYSA-N

Formula: C24H45NO4

SMILES: CCCCCCOC(=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	-204.15	kJ/mol	Joback Method
hf	-962.96	kJ/mol	Joback Method
hfus	49.92	kJ/mol	Joback Method
hvap	88.02	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	6.054		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
pc	935.77	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	922.43	K	Joback Method
tc	1130.41	K	Joback Method
tf	490.93	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.25	J/molxK	922.43	Joback Method
cpg	1288.24	J/molxK	957.09	Joback Method
cpg	1306.50	J/molxK	991.76	Joback Method
cpg	1323.04	J/molxK	1026.42	Joback Method
cpg	1337.91	J/molxK	1061.08	Joback Method
cpg	1351.14	J/molxK	1095.74	Joback Method
cpg	1362.77	J/molxK	1130.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U392413&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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