

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

InChI: InChI=1S/C28H53NO4/c1-8-9-10-11-12-13-14-15-18-32-27(30)25(19-21(2)3)29(7)28(31)
InChIKey: CDMBEENWNOORBL-UHFFFAOYSA-N

Formula: C28H53NO4

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

Mol. weight [g/mol]: 467.72

Physical Properties

Property code	Value	Unit	Source
gf	-170.47	kJ/mol	Joback Method
hf	-1045.52	kJ/mol	Joback Method
hfus	60.28	kJ/mol	Joback Method
hvap	96.92	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.614		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
pc	749.38	kPa	Joback Method
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tb	1013.95	K	Joback Method
tc	1244.80	K	Joback Method
tf	536.01	K	Joback Method
vc	1.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1524.86	J/mol×K	1013.95	Joback Method
cpg	1545.11	J/mol×K	1052.42	Joback Method
cpg	1563.14	J/mol×K	1090.90	Joback Method
cpg	1579.00	J/mol×K	1129.37	Joback Method
cpg	1592.75	J/mol×K	1167.85	Joback Method
cpg	1604.46	J/mol×K	1206.32	Joback Method
cpg	1614.19	J/mol×K	1244.80	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=U392417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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