L-Leucine, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C13H26N2O2/c1-6-7-8-17-13(16)12(9-11(2)3)14-10-15(4)5/h10-12H,6-9H2,1-5

InchiKey: APXKMZSISJFVOJ-UHFFFAOYSA-N

Formula: C13H26N2O2

SMILES: CCCCOC(=O)C(CC(C)C)N=CN(C)C

Mol. weight [g/mol]: 242.36

Physical Properties

Property code	Value	Unit	Source
hf	-417.26	kJ/mol	Joback Method
hvap	58.27	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.334		Crippen Method
mcvol	217.130	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	661.37	K	Joback Method
tc	848.60	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375624&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation 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