l-Leucine, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C15H27NO3/c1-11(2)10-13(15(18)19-3)16-14(17)9-8-12-6-4-5-7-12/h11-13H,4

InchiKey: JNEWIBUQLCHVIJ-UHFFFAOYSA-N

Formula: C15H27NO3

SMILES: COC(=O)C(CC(C)C)N=C(O)CCC1CCCC1

Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
hf	-627.61	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.501		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	802.03	K	Joback Method
tc	1003.45	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299653&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