Propanamide, 3-cyclopentyl-N-hexyl-

Inchi: InChI=1S/C14H27NO/c1-2-3-4-7-12-15-14(16)11-10-13-8-5-6-9-13/h13H,2-12H2,1H3,(H
InchiKey: IWWREQWCCHZILU-UHFFFAOYSA-N
Formula: C14H27NO
SMILES: CCCCCCN=C(O)CCC1CCCC1
Mol. weight [g/mol]: 225.37

Physical Properties

Property code	Value	Unit	Source
hf	-351.61	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.494		Crippen Method
mcvol	208.810	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook
tb	703.74	K	Joback Method
tc	894.19	K	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=U407380&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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