Propanamide, 3-cyclopentyl-N-(3-methylbutyl)-

Inchi: InChI=1S/C13H25NO/c1-11(2)9-10-14-13(15)8-7-12-5-3-4-6-12/h11-12H,3-10H2,1-2H3,(
InchiKey: XNQBVSYWCRFODW-UHFFFAOYSA-N
Formula: C13H25NO
SMILES: CC(C)CCN=C(O)CCC1CCCC1
Mol. weight [g/mol]: 211.34

Physical Properties

Property code	Value	Unit	Source
hf	-336.25	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.959		Crippen Method
mcvol	194.720	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
tb	680.42	K	Joback Method
tc	875.38	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=U407377&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