Propanamide, 3-cyclopentyl-N-isobutyl-

Inchi: InChI=1S/C12H23NO/c1-10(2)9-13-12(14)8-7-11-5-3-4-6-11/h10-11H,3-9H2,1-2H3,(H,13

InchiKey: KSZTXWMYMBKTEP-UHFFFAOYSA-N

Formula: C12H23NO

SMILES: CC(C)CN=C(O)CCC1CCCC1

Mol. weight [g/mol]: 197.32

Physical Properties

Property code	Value	Unit	Source
hf	-315.61	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.569		Crippen Method
mcvol	180.630	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1664.00		NIST Webbook
tb	657.54	K	Joback Method
tc	854.60	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407375&Units=SI

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

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