

Propanamide, 3-cyclopentyl-N-butyl-

Inchi: InChI=1S/C12H23NO/c1-2-3-10-13-12(14)9-8-11-6-4-5-7-11/h11H,2-10H2,1H3,(H,13,14)
InchiKey: WUIJSBHXNFWKQZ-UHFFFAOYSA-N
Formula: C12H23NO
SMILES: CCCCNC(=O)CCC1CCCC1
Mol. weight [g/mol]: 197.32

Physical Properties

Property code	Value	Unit	Source
hf	-310.33	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.713		Crippen Method
mcvol	180.630	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1717.00		NIST Webbook
tb	657.98	K	Joback Method
tc	851.71	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U407376&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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