1-Cyclopropanecarboxamide, 2-phenyl-N-butyl-

Inchi: InChI=1S/C14H19NO/c1-2-3-9-15-14(16)13-10-12(13)11-7-5-4-6-8-11/h4-8,12-13H,2-3,9

InchiKey: SATJMTLQGXWOPT-UHFFFAOYSA-N

Formula: C14H19NO

SMILES: CCCCN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
hf	-123.10	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.547		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	2094.00		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	717.21	K	Joback Method
tc	928.53	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415235&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