1-Cyclopropanecarboxamide, 2-phenyl-N-isobutyl-

Inchi: InChI=1S/C14H19NO/c1-10(2)9-15-14(16)13-8-12(13)11-6-4-3-5-7-11/h3-7,10,12-13H,8-

InchiKey: ZTMXNWWGYHNZLM-UHFFFAOYSA-N

Formula: C14H19NO

SMILES: CC(C)CN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
hf	-128.38	kJ/mol	Joback Method
hvap	68.32	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.403		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	716.77	K	Joback Method
tc	931.74	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=U415234&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