1-Cyclopropanecarboxamide, 2-phenyl-N-pentyl-

Inchi: InChI=1S/C15H21NO/c1-2-3-7-10-16-15(17)14-11-13(14)12-8-5-4-6-9-12/h4-6,8-9,13-14

InchiKey: GBSXFTQPXFAQBC-UHFFFAOYSA-N

Formula: C15H21NO

SMILES: CCCCCN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 231.33

Physical Properties

Property code	Value	Unit	Source
hf	-143.74	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.937		Crippen Method
mcvol	199.140	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	740.09	K	Joback Method
tc	948.81	K	Joback Method

Sources

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=U415237&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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