1-Cyclopropanecarboxamide, 2-phenyl-N-hexyl-

Inchi: InChI=1S/C16H23NO/c1-2-3-4-8-11-17-16(18)15-12-14(15)13-9-6-5-7-10-13/h5-7,9-10,1

InchiKey: PXGCWKFAOBRYAR-UHFFFAOYSA-N

Formula: C16H23NO

SMILES: CCCCCCN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 245.36

Physical Properties

Property code	Value	Unit	Source
hf	-164.38	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.327		Crippen Method
mcvol	213.230	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
tb	762.97	K	Joback Method
tc	969.57	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=U415239&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