

1-Cyclopropanecarboxamide, 2-phenyl-N-propyl-

Inchi:	InChI=1S/C13H17NO/c1-2-8-14-13(15)12-9-11(12)10-6-4-3-5-7-10/h3-7,11-12H,2,8-9H2
InchiKey:	AVQDACOFTDAGII-UHFFFAOYSA-N
Formula:	C13H17NO
SMILES:	CCCN=C(O)C1CC1c1ccccc1
Mol. weight [g/mol]:	203.28

Physical Properties

Property code	Value	Unit	Source
hf	-102.46	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	3.157		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	694.33	K	Joback Method
tc	908.70	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415233&Units=SI
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

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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