1-Cyclopropanecarboxamide, 2-phenyl-N-heptyl-

Inchi: InChI=1S/C17H25NO/c1-2-3-4-5-9-12-18-17(19)16-13-15(16)14-10-7-6-8-11-14/h6-8,10-

InchiKey: TXOMTHRKLJOQFN-UHFFFAOYSA-N

Formula: C17H25NO

SMILES: CCCCCCCN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 259.39

Physical Properties

Property code	Value	Unit	Source
hf	-185.02	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.717		Crippen Method
mcvol	227.320	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	785.85	K	Joback Method
tc	990.87	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415241&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