1-Cyclopropanecarboxamide, 2-phenyl-N-octadecyl-

Inchi: InChI=1S/C28H47NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-29-28(30)27-24-2

InchiKey: QTVQYYOIYKQQJL-UHFFFAOYSA-N

Formula: C28H47NO

SMILES: CCCCCCCCCCCCCCCCCCN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 413.68

Physical Properties

Property code	Value	Unit	Source
hf	-412.06	kJ/mol	Joback Method
hvap	99.87	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	9.008		Crippen Method
mcvol	382.310	ml/mol	McGowan Method
pc	822.90	kPa	Joback Method
rinpol	1544.00		NIST Webbook
rinpol	1544.00		NIST Webbook
tb	1037.53	K	Joback Method
tc	1274.76	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415249&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