1-Cyclopropanecarboxamide, 2-phenyl-N-undecyl-

Inchi: InChI=1S/C21H33NO/c1-2-3-4-5-6-7-8-9-13-16-22-21(23)20-17-19(20)18-14-11-10-12-15

InchiKey: GMMWISKXBBYETA-UHFFFAOYSA-N

Formula: C21H33NO

SMILES: CCCCCCCCCCCN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 315.49

Physical Properties

Property code	Value	Unit	Source
hf	-267.58	kJ/mol	Joback Method
hvap	84.29	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	6.277		Crippen Method
mcvol	283.680	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	3039.00		NIST Webbook
rinpol	3039.00		NIST Webbook
tb	877.37	K	Joback Method
tc	1082.29	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=U415245&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