1-Cyclopropanecarboxamide, 2-phenyl-N-2-ethylhexyl-

Inchi: InChI=1S/C18H27NO/c1-3-5-9-14(4-2)13-19-18(20)17-12-16(17)15-10-7-6-8-11-15/h6-8,

InchiKey: XEKUCLNMSCRIHJ-UHFFFAOYSA-N

Formula: C18H27NO

SMILES: CCCCC(CC)CN=C(O)C1CC1c1ccccc1

Mol. weight [g/mol]: 273.41

Physical Properties

Property code	Value	Unit	Source
hf	-210.94	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.963		Crippen Method
mcvol	241.410	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	808.29	K	Joback Method
tc	1014.77	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=U415240&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