Propanamide, 3-phenyl-N-undecyl-

Inchi: InChI=1S/C20H33NO/c1-2-3-4-5-6-7-8-9-13-18-21-20(22)17-16-19-14-11-10-12-15-19/h1
InchiKey: YJXVGBVPFPEOCQ-UHFFFAOYSA-N
Formula: C20H33NO
SMILES: CCCCCCCCCCCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 303.48

Physical Properties

Property code	Value	Unit	Source
hf	-299.40	kJ/mol	Joback Method
hvap	82.46	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.107		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	852.42	K	Joback Method
tc	1050.84	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407158&Units=SI

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