Propanamide, 3-phenyl-N-pentyl-

Inchi: InChI=1S/C14H21NO/c1-2-3-7-12-15-14(16)11-10-13-8-5-4-6-9-13/h4-6,8-9H,2-3,7,10-1
InchiKey: YOABAXQNDFFNSO-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
hf	-175.56	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.766		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	715.14	K	Joback Method
tc	915.31	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407152&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

Latest version available from:

https://www.chemeo.com/cid/82-636-5/Propanamide-3-phenyl-N-pentyl.pdf

Generated by Cheméo on 2024-10-12 09:11:09.602552707 +0000 UTC m=+3305132.239521965.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.