Benzamide, 2-methyl-N-hexyl-

Inchi: InChI=1S/C14H21NO/c1-3-4-5-8-11-15-14(16)13-10-7-6-9-12(13)2/h6-7,9-10H,3-5,8,11H
InchiKey: WQMHAGWLXHVQEB-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCCCN=C(O)c1ccccc1C
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
hf	-187.03	kJ/mol	Joback Method
hvap	69.77	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.880		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	720.12	K	Joback Method
tc	921.11	K	Joback Method

Sources

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=U407398&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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