Benzamide, 2-methyl-N-pentyl-

Inchi: InChI=1S/C13H19NO/c1-3-4-7-10-14-13(15)12-9-6-5-8-11(12)2/h5-6,8-9H,3-4,7,10H2,1-
InchiKey: DQUVNPQVXDGAJO-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CCCCCN=C(O)c1ccccc1C
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
hf	-166.39	kJ/mol	Joback Method
hvap	67.54	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.490		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
tb	697.24	K	Joback Method
tc	900.40	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=U407396&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