Benzamide, 3-methyl-N-hexyl-

Inchi: InChI=1S/C14H21NO/c1-3-4-5-6-10-15-14(16)13-9-7-8-12(2)11-13/h7-9,11H,3-6,10H2,1
InchiKey: YDRYQLGZSXFHEP-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCCCN=C(O)c1cccc(C)c1
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	1975.00		NIST Webbook
rinpol	1975.00		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=U407415&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

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