Benzamide, N-(1-methylhexyl)-

Inchi: InChI=1S/C14H21NO/c1-3-4-6-9-12(2)15-14(16)13-10-7-5-8-11-13/h5,7-8,10-12H,3-4,6,9
InchiKey: WRVRHPTWOJUQQH-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCCC(C)N=C(O)c1ccccc1
Mol. weight [g/mol]: 219.32
CAS: 105452-89-9

Physical Properties

Property code	Value	Unit	Source
hf	-180.84	kJ/mol	Joback Method
hvap	68.72	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.960		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	714.70	K	Joback Method
tc	918.04	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=C105452899&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

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