

N,N-Dimethyl-N'-benzyl-isobutyramidine

Inchi: InChI=1S/C13H20N2/c1-11(2)13(15(3)4)14-10-12-8-6-5-7-9-12/h5-9,11H,10H2,1-4H3/b1
InchiKey: QSNPIRQLTDEVQK-BUHFOSPRSA-N
Formula: C13H20N2
SMILES: CC(C)C(=NCc1ccccc1)N(C)C
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
hf	59.56	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.803		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1561.00		NIST Webbook
tb	612.08	K	Joback Method
tc	829.80	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162595&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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