N,N-Dimethyl-N'-benzyl-propionamidine

Inchi: InChI=1S/C12H18N2/c1-4-12(14(2)3)13-10-11-8-6-5-7-9-11/h5-9H,4,10H2,1-3H3/b13-12
InchiKey: GTOOPRWBIUWQHJ-OUKQBFOZSA-N
Formula: C12H18N2
SMILES: CCC(=NCc1ccccc1)N(C)C
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
hf	85.48	kJ/mol	Joback Method
hvap	50.02	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.557		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1617.00		NIST Webbook
tb	589.64	K	Joback Method
tc	806.67	K	Joback Method

Sources

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=R162000&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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