

N,N-Dimethyl-N'-phenyl-propionamide

Inchi: InChI=1S/C11H16N2/c1-4-11(13(2)3)12-10-8-6-5-7-9-10/h5-9H,4H2,1-3H3
InchiKey: CJCCZDVSXHPVKQ-UHFFFAOYSA-N
Formula: C11H16N2
SMILES: CCC(=Nc1ccccc1)N(C)C
Mol. weight [g/mol]: 176.26

Physical Properties

Property code	Value	Unit	Source
hf	106.12	kJ/mol	Joback Method
hvap	47.79	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.688		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1510.00		NIST Webbook
tb	566.76	K	Joback Method
tc	787.69	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162095&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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