

N,N-Dimethyl-N'-phenyl-pivalamide

Inchi: InChI=1S/C13H20N2/c1-13(2,3)12(15(4)5)14-11-9-7-6-8-10-11/h6-10H,1-5H3/b14-12+
InchiKey: XQBGYQJKTQCGCJ-WYMLVPIESA-N
Formula: C13H20N2
SMILES: CN(C)C(=Nc1ccccc1)C(C)(C)C
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
hf	56.09	kJ/mol	Joback Method
hvap	50.95	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.324		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1539.00		NIST Webbook
tb	609.29	K	Joback Method
tc	835.50	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=R162788&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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