N,N-Dimethyl-N'-(4-nitrophenyl)-pivalamidine

Inchi: InChI=1S/C13H19N3O2/c1-13(2,3)12(15(4)5)14-10-6-8-11(9-7-10)16(17)18/h6-9H,1-5H3
InchiKey: WHUWWSOADACHNY-WYMLVPIESA-N
Formula: C13H19N3O2
SMILES: CN(C)C(=Nc1ccc([N+](=O)[O-])cc1)C(C)(C)C
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
hf	33.86	kJ/mol	Joback Method
hvap	68.20	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.232		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	2120.00		NIST Webbook
tb	766.11	K	Joback Method
tc	1013.05	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R162580&Units=SI
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

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