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

Inchi: InChI=1S/C12H17N3O2/c1-9(2)12(14(3)4)13-10-5-7-11(8-6-10)15(16)17/h5-9H,1-4H3/b1
InchiKey: ORPMAAUFXHHLID-OUKQBFOZSA-N
Formula: C12H17N3O2
SMILES: CC(C)C(=Nc1ccc([N+](=O)[O-])cc1)N(C)C
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
hf	57.97	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.842		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	746.02	K	Joback Method
tc	989.34	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=R162575&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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