N,N-Dimethyl-N'-(3-nitrophenyl)-propionamidine

Inchi: InChI=1S/C11H15N3O2/c1-4-11(13(2)3)12-9-6-5-7-10(8-9)14(15)16/h5-8H,4H2,1-3H3/b1
InchiKey: GXIUOIPWQGCNTA-VAWYXSNFSA-N
Formula: C11H15N3O2
SMILES: CCC(=Nc1cccc([N+](=O)[O-])c1)N(C)C
Mol. weight [g/mol]: 221.26

Physical Properties

Property code	Value	Unit	Source
hf	83.89	kJ/mol	Joback Method
hvap	65.05	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.596		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	723.58	K	Joback Method
tc	967.21	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=R161938&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