N'-(4-nitro-phenyl)-N,N-dimethyl-acetamidine

Inchi: InChI=1S/C10H13N3O2/c1-8(12(2)3)11-9-4-6-10(7-5-9)13(14)15/h4-7H,1-3H3
InchiKey: SZXZMKAOUGQCFZ-UHFFFAOYSA-N
Formula: C10H13N3O2
SMILES: CC(=Nc1ccc([N+](=O)[O-])cc1)N(C)C
Mol. weight [g/mol]: 207.23

Physical Properties

Property code	Value	Unit	Source
hf	104.53	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.206		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
tb	700.70	K	Joback Method
tc	949.66	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=R153472&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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