N''-(3-nitro-phenyl)-N,N,N',N'-tetramethyl -guanidine

Inchi: InChI=1S/C11H16N4O2/c1-13(2)11(14(3)4)12-9-6-5-7-10(8-9)15(16)17/h5-8H,1-4H3
InchiKey: XRESPTDFWCEXMZ-UHFFFAOYSA-N
Formula: C11H16N4O2
SMILES: CN(C)C(=Nc1cccc([N+](=O)[O-])c1)N(C)C
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
hf	151.42	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.706		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	736.02	K	Joback Method
tc	975.76	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=R153016&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