

(CH3)2N-CH=N-(4-nitrophenyl)

Other names:	Formamidine, 3,3-dimethyl-1-(4-nitrophenyl) Formamidine, N,N-dimethyl-N'-(p-nitrophenyl)- N'-(4-nitro-phenyl)-N,N-dimethyl-formamidine N'-(p-Nitrophenyl)-N,N-dimethylformamidine N,N-Dimethyl-N'-(p-nitrophenyl)formamidine
Inchi:	InChI=1S/C9H11N3O2/c1-11(2)7-10-8-3-5-9(6-4-8)12(13)14/h3-7H,1-2H3
InchiKey:	VBHAVCCSDMDOCP-UHFFFAOYSA-N
Formula:	C9H11N3O2
SMILES:	CN(C)C=Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	193.20
CAS:	74739-51-8

Physical Properties

Property code	Value	Unit	Source
affp	950.20	kJ/mol	NIST Webbook
basg	917.80	kJ/mol	NIST Webbook
hf	134.96	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
ie	7.90 ± 0.10	eV	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.816		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	677.94	K	Joback Method
tc	928.14	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=C1205590&Units=SI

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.chemeo.com/cid/15-011-2/CH3-2N-CH-N-4-nitrophenyl.pdf>

Generated by Cheméo on 2025-12-05 10:11:25.025979314 +0000 UTC m=+4677682.556019979.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.