

# N,N-Dimethyl-N'-(3-nitrophenyl)-p-methylbenzami

**Inchi:** InChI=1S/C16H17N3O2/c1-12-7-9-13(10-8-12)16(18(2)3)17-14-5-4-6-15(11-14)19(20)21  
**InchiKey:** YYCMUEFRWIKHAC-UHFFFAOYSA-N  
**Formula:** C16H17N3O2  
**SMILES:** Cc1ccc(C(=Nc2cccc([N+](=O)[O-])c2)N(C)C)cc1  
**Mol. weight [g/mol]:** 283.33

## Physical Properties

Property code	Value	Unit	Source
hf	205.75	kJ/mol	Joback Method
hvap	79.11	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.543		Crippen Method
mcvol	221.860	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	2341.00		NIST Webbook
tb	869.64	K	Joback Method
tc	1131.49	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158808&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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