

# N,N-Dimethyl-2,2-bis-(2-nitro-phenyl)-acetamide

**Inchi:** InChI=1S/C16H15N3O5/c1-17(2)16(20)15(11-7-3-5-9-13(11)18(21)22)12-8-4-6-10-14(12)  
**InchiKey:** NGPZUAHQOLTERS-UHFFFAOYSA-N  
**Formula:** C16H15N3O5  
**SMILES:** CN(C)C(=O)C(c1ccccc1[N+](=O)[O-])c1ccccc1[N+](=O)[O-]  
**Mol. weight [g/mol]:** 329.31

## Physical Properties

Property code	Value	Unit	Source
gf	339.92	kJ/mol	Joback Method
hf	4.70	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	2.723		Crippen Method
mcvol	235.170	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	2497.00		NIST Webbook
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	998.35	K	Joback Method
tc	1268.64	K	Joback Method
tf	702.58	K	Joback Method
vc	0.897	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.31	J/molxK	998.35	Joback Method
cpg	731.32	J/molxK	1043.40	Joback Method
cpg	740.29	J/molxK	1088.45	Joback Method
cpg	748.38	J/molxK	1133.49	Joback Method
cpg	755.71	J/molxK	1178.54	Joback Method
cpg	762.42	J/molxK	1223.59	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R277791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R277791&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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