

N,N-Dimethyl-2-phenyl-N'-(4-nitrophenyl)-acetami

Inchi:	InChI=1S/C16H17N3O2/c1-18(2)16(12-13-6-4-3-5-7-13)17-14-8-10-15(11-9-14)19(20)21
InchiKey:	ICQLVFUAPULLRO-WUKNDPDISA-N
Formula:	C16H17N3O2
SMILES:	CN(C)C(Cc1ccccc1)=Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	283.33

Physical Properties

Property code	Value	Unit	Source
hf	217.22	kJ/mol	Joback Method
hvap	78.45	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.429		Crippen Method
mcvol	221.860	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	864.66	K	Joback Method
tc	1125.85	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=R162233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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