N,N-Dimethyl-2-(4-nitro-phenyl)-2-phenyl-acetami

Inchi: InChI=1S/C16H16N2O3/c1-17(2)16(19)15(12-6-4-3-5-7-12)13-8-10-14(11-9-13)18(20)21
InchiKey: CPJQCZRPEWVBCC-UHFFFAOYSA-N
Formula: C16H16N2O3
SMILES: CN(C)C(=O)C(c1ccccc1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 284.31

Physical Properties

Property code	Value	Unit	Source
gf	314.00	kJ/mol	Joback Method
hf	26.93	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	2.815		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2449.00		NIST Webbook
rinpol	2446.00		NIST Webbook
rinpol	2449.00		NIST Webbook
tb	841.53	K	Joback Method
tc	1096.81	K	Joback Method
tf	546.45	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.30	J/mol×K	841.53	Joback Method
cpg	647.79	J/mol×K	884.08	Joback Method
cpg	660.02	J/mol×K	926.62	Joback Method
cpg	671.11	J/mol×K	969.17	Joback Method
cpg	681.19	J/mol×K	1011.71	Joback Method
cpg	690.36	J/mol×K	1054.26	Joback Method

cpg	698.74	J/mol×K	1096.81	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=R277875&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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