

N1N1-dimethyl-N2-ortho-nitrophenylformamide

Inchi: InChI=1S/C9H11N3O2/c1-11(2)7-10-8-5-3-4-6-9(8)12(13)14/h3-7H,1-2H3/b10-7+
InchiKey: UBNRMJZJEMXNRG-JXMROGBWSA-N
Formula: C9H11N3O2
SMILES: CN(C)C=Nc1cccc1[N+](=O)[O-]
Mol. weight [g/mol]: 193.20

Physical Properties

Property code	Value	Unit	Source
hf	134.96	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.816		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1784.00		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=R164026&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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