(CH3)2N-CH=N-(4-nitrophenyl)

Inchi: InChI=1S/C9H11N3O2/c1-11(2)7-10-8-3-5-9(6-4-8)12(13)14/h3-7H,1-2H3/b10-7+
InchiKey: VBLAVCCSDMDOCP-JXMROGBWSA-N
Formula: C9H11N3O2
SMILES: CN(C)C=Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 193.20
CAS: 74739-51-8

Physical Properties

Property code	Value	Unit	Source
affp	950.20	kJ/mol	NIST Webbook
basg	917.80	kJ/mol	NIST Webbook
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
tb	677.94	K	Joback Method
tc	928.14	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C74739518&Units=SI

Legend

affp: Proton affinity

basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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