Methanimine, 1-(1-pyrrolidinyl), N-(3-nitrophenyl)

Inchi: InChI=1S/C11H13N3O2/c15-14(16)11-5-3-4-10(8-11)12-9-13-6-1-2-7-13/h3-5,8-9H,1-2,6

InchiKey: NDDHFPHNNRWUOX-FMIVXFBMSA-N

Formula: C11H13N3O2

SMILES: O=[N+]([O-])c1cccc(N=CN2CCCC2)c1

Mol. weight [g/mol]: 219.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.350		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118964&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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