

Methanimine, 1-(1-piperidiny), N-(4-nitrophenyl)

Inchi: InChI=1S/C12H15N3O2/c16-15(17)12-6-4-11(5-7-12)13-10-14-8-2-1-3-9-14/h4-7,10H,1-11
InchiKey: IMKBTFOHBYTFCZ-JLHYYAGUSA-N
Formula: C12H15N3O2
SMILES: O=[N+]([O-])c1ccc(N=CN2CCCCC2)cc1
Mol. weight [g/mol]: 233.27

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.32 | | Crippen Method |
| logp | 2.740 | | Crippen Method |
| mcvol | 178.400 | ml/mol | McGowan Method |
| rinpol | 2365.00 | | NIST Webbook |
| rinpol | 2365.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R118820&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-872-9/Methanimine-1-1-piperidiny-N-4-nitrophenyl.pdf>

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