

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

Inchi: InChI=1S/C12H15N3O2/c16-15(17)12-6-4-5-11(9-12)13-10-14-7-2-1-3-8-14/h4-6,9-10H,
InchiKey: SDRKLRASBJMDHV-UHFFFAOYSA-N
Formula: C12H15N3O2
SMILES: O=[N+]([O-])c1cccc(N=CN2CCCCC2)c1
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	2255.00		NIST Webbook
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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=R118771&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/51-345-2/Methanimine-1-1-piperidiny-N-3-nitrophenyl.pdf>

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