Methanimine, 1-(4-morpholino), N-(3-nitrophenyl)

Inchi: InChI=1S/C11H13N3O3/c15-14(16)11-3-1-2-10(8-11)12-9-13-4-6-17-7-5-13/h1-3,8-9H,4-

InchiKey: ZDPOTHCFQATOEX-FMIVXFBMSA-N

Formula: C11H13N3O3

SMILES: O=[N+]([O-])c1cccc(N=CN2CCOCC2)c1

Mol. weight [g/mol]: 235.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	1.587		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
rinpol	2419.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R119165&Units=SI

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

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices