

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
rinpole	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/ci9903071>
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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/29-465-4/Methanimine-1-4-morpholino-N-3-nitrophenyl.pdf>

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