

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

Inchi: InChI=1S/C12H16N2O2/c1-15-12-4-2-3-11(9-12)13-10-14-5-7-16-8-6-14/h2-4,9-10H,5-8H
InchiKey: UZVXUKZGFJMYKX-UHFFFAOYSA-N
Formula: C12H16N2O2
SMILES: COc1cccc(N=CN2CCOCC2)c1
Mol. weight [g/mol]: 220.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	1.687		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R119145&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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