

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

Inchi: InChI=1S/C12H16N2O/c1-11-3-2-4-12(9-11)13-10-14-5-7-15-8-6-14/h2-4,9-10H,5-8H2,1
InchiKey: LCMRQMTZZPFCOW-UHFFFAOYSA-N
Formula: C12H16N2O
SMILES: Cc1cccc(N=CN2CCOCC2)c1
Mol. weight [g/mol]: 204.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Crippen Method
logp	1.987		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R119150&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/42-981-6/Methanimine-1-4-morpholino-N-3-methylphenyl.pdf>

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