

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

Inchi: InChI=1S/C11H13ClN2O/c12-10-2-1-3-11(8-10)13-9-14-4-6-15-7-5-14/h1-3,8-9H,4-7H2
InchiKey: UIZAQBOFXZMFCC-UHFFFAOYSA-N
Formula: C11H13ClN2O
SMILES: Clc1cccc(N=CN2CCOCC2)c1
Mol. weight [g/mol]: 224.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	2.332		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
rinsol	2011.00		NIST Webbook
rinsol	2011.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R119125&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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