

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

Inchi: InChI=1S/C13H18N2O2/c1-2-17-13-5-3-4-12(10-13)14-11-15-6-8-16-9-7-15/h3-5,10-11H
InchiKey: OALOULVNYURTOG-SDNWHVVSQSA-N
Formula: C13H18N2O2
SMILES: CCOc1cccc(N=CN2CCOCC2)c1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	2.077		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=R119130&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/24-016-7/Methanimine-1-4-morpholino-N-3-ethoxyphenyl.pdf>

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