

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

Inchi:	InChI=1S/C11H13BrN2O/c12-10-2-1-3-11(8-10)13-9-14-4-6-15-7-5-14/h1-3,8-9H,4-7H2
InchiKey:	GJNIMZWOSCTCDD-UHFFFAOYSA-N
Formula:	C11H13BrN2O
SMILES:	BrC1CCCC(N=CN2CCOCC2)c1
Mol. weight [g/mol]:	269.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	2.441		Crippen Method
mcvol	170.260	ml/mol	McGowan Method
rinpol	2119.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R119110&Units=SI

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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