# 4-(1,3-Benzothiazol-2-yl)morpholine

**Inchi:** InChI=1S/C11H12N2OS/c1-2-4-10-9(3-1)12-11(15-10)13-5-7-14-8-6-13/h1-4H,5-8H2
**InchiKey:** VVUVJGRVEYHIHC-UHFFFAOYSA-N
**Formula:** C11H12N2OS
**SMILES:** c1ccc2sc(N3CCOCC3)nc2c1
**Mol. weight [g/mol]:** 220.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.53 | | Crippen Method |
| logp | 2.133 | | Crippen Method |
| mcvol | 158.250 | ml/mol | McGowan Method |
| rinpol | 1945.00 | | NIST Webbook |
| rinpol | 1945.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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=R577863&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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