2-(4-Morpholinyl)benzothiazole

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
CAS: 4225-26-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	2.133		Crippen Method
mcvol	158.250	ml/mol	McGowan Method

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=C4225267&Units=SI&Mask=3FFF

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume