

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/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=C4225267&Units=SI&Mask=3FFF

Legend

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

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<https://www.chemeo.com/cid/122-750-3/2-4-Morpholinyl-benzothiazole.pdf>

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