2-(2-Benzothiazolyl)-5-methoxyphenol

Inchi: InChI=1S/C14H11NO2S/c1-17-9-6-7-10(12(16)8-9)14-15-11-4-2-3-5-13(11)18-14/h2-8,1
InchiKey: KQUJPMLQKNTPCL-UHFFFAOYSA-N
Formula: C14H11NO2S
SMILES: COc1ccc(-c2nc3ccccc3s2)c(O)c1
Mol. weight [g/mol]: 257.31
CAS: 90481-46-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	3.677		Crippen Method
mcvol	183.510	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90481462&Units=SI
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

Legend

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