

2-(2-Benzothiazolyl)-5-methylphenol

Inchi:	InChI=1S/C14H11NOS/c1-9-6-7-10(12(16)8-9)14-15-11-4-2-3-5-13(11)17-14/h2-8,16H,1
InchiKey:	DILRSGGQTSJRST-UHFFFAOYSA-N
Formula:	C14H11NOS
SMILES:	Cc1ccc(-c2nc3ccccc3s2)c(O)c1
Mol. weight [g/mol]:	241.31
CAS:	56048-54-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	3.977		Crippen Method
mcvol	177.640	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=C56048545&Units=SI

Legend

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

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