

2-Benzoxazolethiol, 5-phenyl-

Inchi:	InChI=1S/C13H9NOS/c16-13-14-11-8-10(6-7-12(11)15-13)9-4-2-1-3-5-9/h1-8H,(H,14,16)
InchiKey:	QKLMWNVNJBXKRG-UHFFFAOYSA-N
Formula:	C13H9NOS
SMILES:	Sc1nc2cc(-c3ccccc3)ccc2o1
Mol. weight [g/mol]:	227.28
CAS:	17371-99-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.89		Crippen Method
logp	3.784		Crippen Method
mcvol	163.550	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=C17371992&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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