

3-Hydroxy-4-methyl-6-chloro-thionaphthene

Inchi:	InChI=1S/C9H7ClOS/c1-5-2-6(10)3-8-9(5)7(11)4-12-8/h2-4,11H,1H3
InchiKey:	DKYFBPUTEGRWLF-UHFFFAOYSA-N
Formula:	C9H7ClOS
SMILES:	Cc1cc(Cl)cc2scc(O)c12
Mol. weight [g/mol]:	198.67
CAS:	5340-96-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	3.569		Crippen Method
mcvol	133.210	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5340965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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