

4-Hydroxy-4-phenyl-3,5,5-trimethylthiazolidine-2-thione

Inchi:	InChI=1S/C12H15NOS2/c1-11(2)12(14,13(3)10(15)16-11)9-7-5-4-6-8-9/h4-8,14H,1-3H3
InchiKey:	SDCNDOSDKGZCOM-UHFFFAOYSA-N
Formula:	C12H15NOS2
SMILES:	CN1C(=S)SC(C)(C)C1(O)c1ccccc1
Mol. weight [g/mol]:	253.38
CAS:	95982-07-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.574		Crippen Method
mcvol	189.570	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95982073&Units=SI
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

Legend

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

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