

4-[(Hexylsulfonyl)methyl]-4-thiazoline-2-thione

Inchi:	InChI=1S/C10H17NO2S3/c1-2-3-4-5-6-16(12,13)8-9-7-15-10(14)11-9/h7H,2-6,8H2,1H3,
InchiKey:	WRKNEGJMKRHFCQ-UHFFFAOYSA-N
Formula:	C10H17NO2S3
SMILES:	CCCCCCS(=O)(=O)Cc1csc(=S)[nH]1
Mol. weight [g/mol]:	279.44
CAS:	90978-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.819		Crippen Method
mcvol	203.070	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=C90978851&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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