

4-(N-heptylsulfonylmethyl)-4-thiazoline-2-thione

Inchi:	InChI=1S/C11H19NO2S3/c1-2-3-4-5-6-7-17(13,14)9-10-8-16-11(15)12-10/h8H,2-7,9H2,1
InchiKey:	IBXDRHOQOVLHFS-UHFFFAOYSA-N
Formula:	C11H19NO2S3
SMILES:	CCCCCCCS(=O)(=O)Cc1csc(=S)[nH]1
Mol. weight [g/mol]:	293.47
CAS:	91356-11-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	3.209		Crippen Method
mcvol	217.160	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91356115&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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