

(N-pentylsulfonyl) methyl-4-thiazoline-2-thione

Inchi:	InChI=1S/C9H15NO2S3/c1-2-3-4-5-15(11,12)7-8-6-14-9(13)10-8/h6H,2-5,7H2,1H3,(H,10)
InchiKey:	ZXQIGUYJSJISFD-UHFFFAOYSA-N
Formula:	C9H15NO2S3
SMILES:	CCCCCS(=O)(=O)Cc1csc(=S)[nH]1
Mol. weight [g/mol]:	265.42
CAS:	90942-87-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	2.429		Crippen Method
mcvol	188.980	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=C90942873&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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