(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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90942873&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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