

Bis-(n-pentanesulfonyl methyl)-2-thiazolyl disulfide

Inchi:	InChI=1S/C18H28N2O4S6/c1-3-5-7-9-29(21,22)13-15-11-25-17(19-15)27-28-18-20-16(1
InchiKey:	YZNBNJKXZNVMBJ-UHFFFAOYSA-N
Formula:	C18H28N2O4S6
SMILES:	CCCCCS(=O)(=O)Cc1csc(SSc2nc(CS(=O)(=O)CCCC)cs2)n1
Mol. weight [g/mol]:	528.82
CAS:	93999-94-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.42		Crippen Method
logp	5.609		Crippen Method
mcvol	367.100	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=C93999941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/25-547-7/Bis-n-pentanesulfonyl-methyl-2-thiazolyl-disulfide.pdf>

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