

2,2'-Bis [(4-n-propylsulfonylmethyl)thiazolyl] disulfide

Inchi:	InChI=1S/C14H20N2O4S6/c1-3-5-25(17,18)9-11-7-21-13(15-11)23-24-14-16-12(8-22-14
InchiKey:	IMMMPJNZFFXZFH-UHFFFAOYSA-N
Formula:	C14H20N2O4S6
SMILES:	CCCS(=O)(=O)Cc1csc(SSc2nc(CS(=O)(=O)CCC)cs2)n1
Mol. weight [g/mol]:	472.71
CAS:	92375-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	4.049		Crippen Method
mcvol	310.740	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=C92375230&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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