

2,2'-Dithio bis 4-(n-heptylsulfonylmethyl)thiazole

Inchi:	InChI=1S/C22H36N2O4S6/c1-3-5-7-9-11-13-33(25,26)17-19-15-29-21(23-19)31-32-22-2
InchiKey:	GEHXEIRCTSIGCZ-UHFFFAOYSA-N
Formula:	C22H36N2O4S6
SMILES:	CCCCCCS(=O)(=O)Cc1csc(SSc2nc(CS(=O)(=O)CCCCC)cs2)n1
Mol. weight [g/mol]:	584.92
CAS:	95288-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.09		Crippen Method
logp	7.169		Crippen Method
mcvol	423.460	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=C95288827&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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