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: CCCCCCCS(=O)(=O)Cc1csc(SSc2nc(CS(=O)(=O)CCCCCCC)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/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