5,5'-Bis-benzylmercapto-[2,2'-azo-1,3,4-thiadiazol]

Inchi: InChI=1S/C18H14N6S4/c1-3-7-13(8-4-1)11-25-17-23-21-15(27-17)19-20-16-22-24-18(28

InchiKey: WIKBHKKLPKRXTP-FMQUCBEESA-N

Formula: C18H14N6S4

SMILES: c1ccc(CSc2nnc(N=Nc3nnc(SCc4ccccc4)s3)s2)cc1

Mol. weight [g/mol]: 442.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	6.390		Crippen Method
mcvol	299.020	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003628&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume