Disulfide, bis[n(benzothiazol-2-yl)-2-aminoethyl]

Inchi: InChI=1S/C18H18N4S4/c1-3-7-15-13(5-1)21-17(25-15)19-9-11-23-24-12-10-20-18-22-14

InchiKey: BFRPCSUPHDDASD-UHFFFAOYSA-N

Formula: C18H18N4S4

SMILES: c1ccc2sc(NCCSSCCNc3nc4ccccc4s3)nc2c1

Mol. weight [g/mol]: 418.62

CAS: 98782-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.39		Crippen Method
logp	5.811		Crippen Method
mcvol	291.960	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=C98782060&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