

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

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