

4,4'-Dibenzyl-[2,2'-azo-1,3,4-thiadiazol-5-one]

Inchi:	InChI=1S/C18H14N6O2S2/c25-17-23(11-13-7-3-1-4-8-13)21-15(27-17)19-20-16-22-24(1
InchiKey:	OHBFGUBBDBYEPD-FMQUCBEESA-N
Formula:	C18H14N6O2S2
SMILES:	O=c1sc(N=Nc2nn(Cc3ccccc3)c(=O)s2)nn1Cc1ccccc1
Mol. weight [g/mol]:	410.47
CAS:	109511-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.435		Crippen Method
mcvol	278.060	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=C109511037&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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