5,5'-Diphenyl-[2,2'-azo-1,3,4-thiadiazole]

Inchi: InChI=1S/C16H10N6S2/c1-3-7-11(8-4-1)13-17-19-15(23-13)21-22-16-20-18-14(24-16)12
InchiKey: FGLPRSIDBGZJGS-QURGRASLSA-N
Formula: C16H10N6S2
SMILES: c1ccc(-c2nnc(N=Nc3nnc(-c4ccccc4)s3)s2)cc1
Mol. weight [g/mol]: 350.42
CAS: 101279-08-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	5.139		Crippen Method
mcvol	238.140	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101279087&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:
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