

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

Inchi:	InChI=1S/C4Cl2N6S2/c5-1-7-9-3(13-1)11-12-4-10-8-2(6)14-4/b12-11+
InchiKey:	QGAVOHHIQXJMTC-VAWYXSNFSA-N
Formula:	C4Cl2N6S2
SMILES:	Clc1nnc(N=Nc2nnc(Cl)s2)s1
Mol. weight [g/mol]:	267.12
CAS:	98020-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	3.112		Crippen Method
mcvol	141.060	ml/mol	McGowan Method

Sources

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=C98020861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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