

2,2'-Azo-1,3,4-thiadiazol-5-one

Inchi:	InChI=1S/C4H2N6O2S2/c11-3-9-7-1(13-3)5-6-2-8-10-4(12)14-2/h(H,9,11)(H,10,12)/b6-5
InchiKey:	RCXQQQWNJKDIHC-AATRIKPKSA-N
Formula:	C4H2N6O2S2
SMILES:	O=c1[nH]nc(N=Nc2n[nH]c(=O)s2)s1
Mol. weight [g/mol]:	230.23
CAS:	116529-21-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.16		Crippen Method
logp	-0.572		Crippen Method
mcvol	128.320	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=C116529216&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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