

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

<b>Inchi:</b>	InChI=1S/C8H6N6O4S2/c1-3(15)13-7(17)19-5(11-13)9-10-6-12-14(4(2)16)8(18)20-6/h1-
<b>InchiKey:</b>	WEVDGPZETOVFSR-MDZDMXLPSA-N
<b>Formula:</b>	C8H6N6O4S2
<b>SMILES:</b>	CC(=O)n1nc(N=Nc2nn(C(C)=O)c(=O)s2)sc1=O
<b>Mol. weight [g/mol]:</b>	314.30
<b>CAS:</b>	116529-22-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.659		Crippen Method
mcvol	187.820	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116529227&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116529227&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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