

# 3-Acetyl-5-methylmercapto-1,3,4-thiadiazolidone-

<b>Inchi:</b>	InChI=1S/C10H12N6O2S4/c1-5(17)15-7(21-9(13-15)19-3)11-12-8-16(6(2)18)14-10(20-4
<b>InchiKey:</b>	SWODMZIVYYKZKL-NTLHZVPKSA-N
<b>Formula:</b>	C10H12N6O2S4
<b>SMILES:</b>	CSc1nn(C(C)=O)c(=NN=c2sc(SC)nn2C(C)=O)s1
<b>Mol. weight [g/mol]:</b>	376.50
<b>CAS:</b>	109967-13-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	1.383		Crippen Method
mcvol	241.260	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C109967137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109967137&amp;Units=SI</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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