

# 3-Acetyl-5-benzylmercapto-1,3,4-thiadiazolidone-2

<b>Inchi:</b>	InChI=1S/C22H20N6O2S4/c1-15(29)27-19(33-21(25-27)31-13-17-9-5-3-6-10-17)23-24-2
<b>InchiKey:</b>	VOTOPRDWEDFYLS-KDMDJZHMSA-N
<b>Formula:</b>	C22H20N6O2S4
<b>SMILES:</b>	CC(=O)n1nc(SCc2ccccc2)sc1=NN=c1sc(SCc2ccccc2)nn1C(C)=O
<b>Mol. weight [g/mol]:</b>	528.69
<b>CAS:</b>	114383-24-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.58		Crippen Method
logp	4.524		Crippen Method
mcvol	362.820	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=C114383243&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C114383243&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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