

# 5-Benzylmercapto-1,3,4-thiadiazolidone-2-azine

<b>Inchi:</b>	InChI=1S/C18H16N6S4/c1-3-7-13(8-4-1)11-25-17-23-21-15(27-17)19-20-16-22-24-18(28
<b>InchiKey:</b>	KXFVLMVRFHGDDBH-UHFFFAOYSA-N
<b>Formula:</b>	C18H16N6S4
<b>SMILES:</b>	<chem>c1ccc(CSc2n[nH]c(=NN=c3[nH]nc(SCc4ccccc4)s3)s2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	444.62
<b>CAS:</b>	114205-74-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.79		Crippen Method
logp	3.293		Crippen Method
mvol	303.320	ml/mol	McGowan Method

## Sources

<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=C114205742&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C114205742&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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