

# Rhodanine, n-diacetylamino-

<b>Inchi:</b>	InChI=1S/C7H8N2O3S2/c1-4(10)8(5(2)11)9-6(12)3-14-7(9)13/h3H2,1-2H3
<b>InchiKey:</b>	QASDIQBQSQLCHF-UHFFFAOYSA-N
<b>Formula:</b>	C7H8N2O3S2
<b>SMILES:</b>	CC(=O)N(C(C)=O)N1C(=O)CSC1=S
<b>Mol. weight [g/mol]:</b>	232.28
<b>CAS:</b>	20904-81-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	0.157		Crippen Method
mcvol	151.700	ml/mol	McGowan Method

## Sources

<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=C20904818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20904818&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>

## 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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<https://www.chemeo.com/cid/24-294-9/Rhodanine-n-diacetylamino.pdf>

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