

# Rhodanine, 3-benzylideneamino

<b>Inchi:</b>	InChI=1S/C10H8N2OS2/c13-9-7-15-10(14)12(9)11-6-8-4-2-1-3-5-8/h1-6H,7H2/b11-6+
<b>InchiKey:</b>	JSDMGFQHQRBMZJS-IZZDOVSWSA-N
<b>Formula:</b>	C10H8N2OS2
<b>SMILES:</b>	O=C1CSC(=S)N1N=Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	236.31
<b>CAS:</b>	4992-28-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	1.881		Crippen Method
mcvol	162.770	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4992283&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4992283&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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