

# Rhodanine, 5-m-nitrobenzylidene-3-m-nitrobenzylideneamino

<b>Inchi:</b>	InChI=1S/C17H10N4O5S2/c22-16-15(9-11-3-1-5-13(7-11)20(23)24)28-17(27)19(16)18-1
<b>InchiKey:</b>	XQXVZALZZYMHOR-HJSNDYAYSA-N
<b>Formula:</b>	C17H10N4O5S2
<b>SMILES:</b>	O=C1C(=Cc2cccc([N+](=O)[O-])c2)SC(=S)N1N=Cc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	414.42
<b>CAS:</b>	17521-29-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	3.738		Crippen Method
mcvol	268.180	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=C17521298&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17521298&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>mcvol:</b>	McGowan's characteristic volume

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