

# Rhodanine, 5-benzylidene-3-phenyl

<b>Inchi:</b>	InChI=1S/C16H11NOS2/c18-15-14(11-12-7-3-1-4-8-12)20-16(19)17(15)13-9-5-2-6-10-13
<b>InchiKey:</b>	TZPSGDWUSVAMNF-SDNWHVSQSA-N
<b>Formula:</b>	C16H11NOS2
<b>SMILES:</b>	O=C1C(=Cc2ccccc2)SC(=S)N1c1ccccc1
<b>Mol. weight [g/mol]:</b>	297.39
<b>CAS:</b>	13037-56-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.092		Crippen Method
mcvol	213.570	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=C13037564&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13037564&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

Latest version available from:

<https://www.chemeo.com/cid/24-292-1/Rhodanine-5-benzylidene-3-phenyl.pdf>

Generated by Cheméo on 2024-05-05 02:41:51.103538482 +0000 UTC m=+17166160.024115798.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.