

# Rhodanine, 5-p-methoxybenzylidene-

<b>Inchi:</b>	InChI=1S/C11H9NO2S2/c1-14-8-4-2-7(3-5-8)6-9-10(13)12-11(15)16-9/h2-6H,1H3,(H,12,
<b>InchiKey:</b>	ORGCJYCWFZQEFX-RMKNXTFCSA-N
<b>Formula:</b>	C11H9NO2S2
<b>SMILES:</b>	COc1ccc(C=C2SC(=S)NC2=O)cc1
<b>Mol. weight [g/mol]:</b>	251.32
<b>CAS:</b>	5462-97-5

## Physical Properties

Property code	Value	Unit	Source
gf	225.07	kJ/mol	Joback Method
hf	39.79	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.184		Crippen Method
mcvol	172.750	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	768.59	K	Joback Method
tc	1051.91	K	Joback Method
tf	620.77	K	Joback Method
vc	0.615	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.77	J/molxK	768.59	Joback Method
cpg	437.12	J/molxK	815.81	Joback Method
cpg	448.34	J/molxK	863.03	Joback Method
cpg	458.48	J/molxK	910.25	Joback Method
cpg	467.56	J/molxK	957.47	Joback Method
cpg	475.63	J/molxK	1004.69	Joback Method
cpg	482.71	J/molxK	1051.91	Joback 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=C5462975&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5462975&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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