

# Rhodanine, 5-salicylidene-

<b>Inchi:</b>	InChI=1S/C10H7NO2S2/c12-7-4-2-1-3-6(7)5-8-9(13)11-10(14)15-8/h1-5,12H,(H,11,13,14)
<b>InchiKey:</b>	ZROKEZLWNZKNSJ-VMPITWQZSA-N
<b>Formula:</b>	C10H7NO2S2
<b>SMILES:</b>	O=C1NC(=S)SC1=Cc1ccccc1O
<b>Mol. weight [g/mol]:</b>	237.30
<b>CAS:</b>	34709-44-9

## Physical Properties

Property code	Value	Unit	Source
gf	176.66	kJ/mol	Joback Method
hf	26.81	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	78.79	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	1.881		Crippen Method
mcvol	158.660	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
tb	798.93	K	Joback Method
tc	1099.60	K	Joback Method
tf	686.47	K	Joback Method
vc	0.506	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.56	J/molxK	798.93	Joback Method
cpg	401.12	J/molxK	849.04	Joback Method
cpg	411.10	J/molxK	899.15	Joback Method
cpg	420.71	J/molxK	949.26	Joback Method
cpg	430.12	J/molxK	999.37	Joback Method
cpg	439.54	J/molxK	1049.49	Joback Method
cpg	449.16	J/molxK	1099.60	Joback Method

# Sources

<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>
<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=C34709449&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34709449&amp;Units=SI</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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