

# Rhodanine, 5-benzylidene

<b>Inchi:</b>	InChI=1S/C10H7NOS2/c12-9-8(14-10(13)11-9)6-7-4-2-1-3-5-7/h1-6H,(H,11,12,13)/b8-6-
<b>InchiKey:</b>	OONWCXLYKDWKOU-VURMDHGXSA-N
<b>Formula:</b>	C10H7NOS2
<b>SMILES:</b>	OC1=NC(=S)SC1=Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	221.30
<b>CAS:</b>	3806-42-6

## Physical Properties

Property code	Value	Unit	Source
gf	366.45	kJ/mol	Joback Method
hf	269.06	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.016		Crippen Method
mcvol	152.790	ml/mol	McGowan Method
pc	4869.76	kPa	Joback Method
tb	751.96	K	Joback Method
tc	1014.54	K	Joback Method
tf	547.14	K	Joback Method
vc	0.550	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.14	J/molxK	751.96	Joback Method
cpg	381.64	J/molxK	795.72	Joback Method
cpg	390.30	J/molxK	839.49	Joback Method
cpg	398.22	J/molxK	883.25	Joback Method
cpg	405.49	J/molxK	927.02	Joback Method
cpg	412.21	J/molxK	970.78	Joback Method
cpg	418.48	J/molxK	1014.54	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=C3806426&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3806426&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mcvol:</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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