

# Rhodanine, 5-(p-nitrobenzylidene)-

<b>Inchi:</b>	InChI=1S/C10H6N2O3S2/c13-9-8(17-10(16)11-9)5-6-1-3-7(4-2-6)12(14)15/h1-5H,(H,11,
<b>InchiKey:</b>	FRWNAQDBODEVAL-VMPITWQZSA-N
<b>Formula:</b>	C10H6N2O3S2
<b>SMILES:</b>	O=C1NC(=S)SC1=Cc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	266.30
<b>CAS:</b>	4120-64-3

## Physical Properties

Property code	Value	Unit	Source
gf	357.20	kJ/mol	Joback Method
hf	181.89	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.084		Crippen Method
mcvol	170.210	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	875.13	K	Joback Method
tc	1185.79	K	Joback Method
tf	730.88	K	Joback Method
vc	0.623	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.68	J/molxK	875.13	Joback Method
cpg	439.25	J/molxK	926.91	Joback Method
cpg	447.78	J/molxK	978.68	Joback Method
cpg	455.36	J/molxK	1030.46	Joback Method
cpg	462.10	J/molxK	1082.24	Joback Method
cpg	468.10	J/molxK	1134.01	Joback Method
cpg	473.44	J/molxK	1185.79	Joback Method

# Sources

<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=C4120643&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4120643&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>

# 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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