

# 3,4-Dihydroxyphenyl thiocyanate

<b>Inchi:</b>	InChI=1S/C7H5NO2S/c8-4-11-5-1-2-6(9)7(10)3-5/h1-3,9-10H
<b>InchiKey:</b>	VRLFTHKJVNALNA-UHFFFAOYSA-N
<b>Formula:</b>	C7H5NO2S
<b>SMILES:</b>	N#CSc1ccc(O)c(O)c1
<b>Mol. weight [g/mol]:</b>	167.19
<b>CAS:</b>	5393-22-6

## Physical Properties

Property code	Value	Unit	Source
gf	-22.47	kJ/mol	Joback Method
hf	-99.15	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.671		Crippen Method
mcvol	115.200	ml/mol	McGowan Method
pc	6209.79	kPa	Joback Method
tb	718.34	K	Joback Method
tc	992.90	K	Joback Method
tf	517.90	K	Joback Method
vc	0.332	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.51	J/molxK	718.34	Joback Method
cpg	277.02	J/molxK	764.10	Joback Method
cpg	283.22	J/molxK	809.86	Joback Method
cpg	289.30	J/molxK	855.62	Joback Method
cpg	295.45	J/molxK	901.38	Joback Method
cpg	301.87	J/molxK	947.14	Joback Method
cpg	308.73	J/molxK	992.90	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=C5393226&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5393226&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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