

# Isatin, 3-thiosemicarbazone

<b>Other names:</b>	(1,2-dihydro-2-oxo-3H-indol-3-al) thiosemicarbazone
<b>Inchi:</b>	InChI=1S/C9H8N4OS/c10-9(15)13-12-7-5-3-1-2-4-6(5)11-8(7)14/h1-4H,(H3,10,13,15)(H,
<b>InchiKey:</b>	SLEMRAMJSGBARH-UHFFFAOYSA-N
<b>Formula:</b>	C9H8N4OS
<b>SMILES:</b>	NC(=S)NN=C1C(=O)Nc2ccccc21
<b>Mol. weight [g/mol]:</b>	220.25
<b>CAS:</b>	487-16-1

## Physical Properties

Property code	Value	Unit	Source
hf	264.01	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	0.176		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	836.66	K	Joback Method
tc	1118.68	K	Joback Method

## Sources

<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=C487161&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C487161&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>

## Legend

<b>hf:</b>	Enthalpy of formation 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

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