

# Iberin

**Inchi:** InChI=1S/C5H9NOS2/c1-9(7)4-2-3-6-5-8/h2-4H2,1H3  
**InchiKey:** LELAOEBVZLPXAZ-UHFFFAOYSA-N  
**Formula:** C5H9NOS2  
**SMILES:** CS(=O)CCCN=C=S  
**Mol. weight [g/mol]:** 163.26  
**CAS:** 505-44-2

## Physical Properties

Property code	Value	Unit	Source
hf	-68.20	kJ/mol	Joback Method
hvap	49.89	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.858		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	518.03	K	Joback Method
tc	742.76	K	Joback Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C505442&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**hf:** Enthalpy of formation at standard conditions

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>r<sub>inpol</sub>:</b>	Non-polar retention indices
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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