

# cis-Wiskey lactone, thio

Inchi:	InChI=1S/C9H16OS/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8-/m0/s1
InchiKey:	MXJQBWKNBCIJHS-YUMQZZPRSA-N
Formula:	C9H16OS
SMILES:	CCCCC1SC(=O)CC1C
Mol. weight [g/mol]:	172.29

## Physical Properties

Property code	Value	Unit	Source
gf	-28.99	kJ/mol	Joback Method
hf	-281.39	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.845		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1961.00		NIST Webbook
tb	531.58	K	Joback Method
tc	752.96	K	Joback Method
tf	349.52	K	Joback Method
vc	0.532	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.22	J/molxK	531.58	Joback Method
cpg	358.53	J/molxK	568.48	Joback Method
cpg	375.00	J/molxK	605.37	Joback Method
cpg	390.63	J/molxK	642.27	Joback Method
cpg	405.43	J/molxK	679.17	Joback Method
cpg	419.40	J/molxK	716.07	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=R585983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R585983&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<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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