

# 5-(2'-Hydroxybenzylidene)-2-thiohydantoin

<b>Inchi:</b>	InChI=1S/C10H8N2O2S/c13-8-4-2-1-3-6(8)5-7-9(14)12-10(15)11-7/h1-5,13H,(H2,11,12,
<b>InchiKey:</b>	DAJICUYKPNPGQQ-FNORWQNLSA-N
<b>Formula:</b>	C10H8N2O2S
<b>SMILES:</b>	O=C1NC(=S)NC1=Cc1cccc1O
<b>Mol. weight [g/mol]:</b>	220.25
<b>CAS:</b>	636-86-2

## Physical Properties

Property code	Value	Unit	Source
gf	224.51	kJ/mol	Joback Method
hf	19.36	kJ/mol	Joback Method
hfus	39.39	kJ/mol	Joback Method
hvap	79.74	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	0.737		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
tb	799.65	K	Joback Method
tc	1090.76	K	Joback Method
tf	708.05	K	Joback Method
vc	0.497	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.96	J/molxK	799.65	Joback Method
cpg	404.06	J/molxK	848.17	Joback Method
cpg	414.48	J/molxK	896.69	Joback Method
cpg	424.39	J/molxK	945.21	Joback Method
cpg	433.92	J/molxK	993.72	Joback Method
cpg	443.22	J/molxK	1042.24	Joback Method
cpg	452.44	J/molxK	1090.76	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=C636862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C636862&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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