

# 2H-1-Benzothiopyran, 3,4-dihydro-

<b>Other names:</b>	Thiochroman Thiachroman Thiochromane 4H-1-Benzothiopyran, 2,3-dihydro-
<b>Inchi:</b>	InChI=1S/C9H10S/c1-2-6-9-8(4-1)5-3-7-10-9/h1-2,4,6H,3,5,7H2
<b>InchiKey:</b>	WPWNEKFMGCWNPR-UHFFFAOYSA-N
<b>Formula:</b>	C9H10S
<b>SMILES:</b>	<chem>c1ccc2c(c1)CCCS2</chem>
<b>Mol. weight [g/mol]:</b>	150.24
<b>CAS:</b>	2054-35-5

## Physical Properties

Property code	Value	Unit	Source
gf	223.90	kJ/mol	Joback Method
hf	128.21	kJ/mol	Joback Method
hfus	11.34	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
ie	8.02	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.725		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	500.49	K	Joback Method
tc	752.24	K	Joback Method
tf	332.24	K	Joback Method
vc	0.427	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.01	J/mol×K	500.49	Joback Method
cpg	258.17	J/mol×K	542.45	Joback Method
cpg	272.10	J/mol×K	584.41	Joback Method
cpg	284.90	J/mol×K	626.37	Joback Method

cpg	296.65	J/mol×K	668.33	Joback Method
cpg	307.45	J/mol×K	710.28	Joback Method
cpg	317.39	J/mol×K	752.24	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=C2054355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2054355&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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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