

# Thiophene, 2,3-dihydro-2-mercapto-3,4-dimethyl, syn-

Inchi:	InChI=1S/C6H10S2/c1-4-3-8-6(7)5(4)2/h3,5-7H,1-2H3/t5-,6+/m0/s1
InchiKey:	VNWDIRWAEAIKU-NTSWFWBYSAN
Formula:	C6H10S2
SMILES:	CC1=CSC(S)C1C
Mol. weight [g/mol]:	146.27

## Physical Properties

Property code	Value	Unit	Source
gf	118.06	kJ/mol	Joback Method
hf	3.02	kJ/mol	Joback Method
hfus	14.83	kJ/mol	Joback Method
hvap	42.40	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.529		Crippen Method
mvol	112.940	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1106.00		NIST Webbook
tb	462.12	K	Joback Method
tc	705.66	K	Joback Method
tf	297.23	K	Joback Method
vc	0.398	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.07	J/mol×K	462.12	Joback Method
cpg	229.33	J/mol×K	502.71	Joback Method
cpg	241.81	J/mol×K	543.30	Joback Method
cpg	253.53	J/mol×K	583.89	Joback Method
cpg	264.52	J/mol×K	624.48	Joback Method
cpg	274.80	J/mol×K	665.07	Joback Method
cpg	284.41	J/mol×K	705.66	Joback Method

# Sources

<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>
<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=R69390&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R69390&amp;Units=SI</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>rinpola:</b>	Non-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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