

# 3-Methyl-3H-1,2-dithiole

Inchi:	InChI=1S/C4H6S2/c1-4-2-3-5-6-4/h2-4H,1H3
InchiKey:	NKTXJFKBFZWDLD-UHFFFAOYSA-N
Formula:	C4H6S2
SMILES:	CC1C=CSS1
Mol. weight [g/mol]:	118.22
CAS:	118023-96-4

## Physical Properties

Property code	Value	Unit	Source
gf	129.03	kJ/mol	Joback Method
hf	82.89	kJ/mol	Joback Method
hfus	8.59	kJ/mol	Joback Method
hvap	36.67	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.284		Crippen Method
mcpol	84.760	ml/mol	McGowan Method
pc	5116.65	kPa	Joback Method
rinpol	1058.80		NIST Webbook
rinpol	1058.80		NIST Webbook
rinpol	1058.80		NIST Webbook
tb	401.02	K	Joback Method
tc	639.88	K	Joback Method
tf	313.40	K	Joback Method
vc	0.279	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.70	J/molxK	401.02	Joback Method
cpg	146.62	J/molxK	440.83	Joback Method
cpg	155.85	J/molxK	480.64	Joback Method
cpg	164.43	J/molxK	520.45	Joback Method
cpg	172.40	J/molxK	560.26	Joback Method
cpg	179.79	J/molxK	600.07	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=C118023964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C118023964&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>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>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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