

# 3,6-Dimethyl-1,2-dithian-4-one

<b>Inchi:</b>	InChI=1S/C6H10OS2/c1-4-3-6(7)5(2)9-8-4/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	AIYPIRMRRSFZEP-UHFFFAOYSA-N
<b>Formula:</b>	C6H10OS2
<b>SMILES:</b>	CC1CC(=O)C(C)SS1
<b>Mol. weight [g/mol]:</b>	162.27

## Physical Properties

Property code	Value	Unit	Source
gf	-26.49	kJ/mol	Joback Method
hf	-180.37	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	44.94	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.118		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinsol	1274.00		NIST Webbook
tb	515.04	K	Joback Method
tc	772.76	K	Joback Method
tf	395.64	K	Joback Method
vc	0.403	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.18	J/mol×K	515.04	Joback Method
cpg	266.35	J/mol×K	557.99	Joback Method
cpg	280.73	J/mol×K	600.95	Joback Method
cpg	294.30	J/mol×K	643.90	Joback Method
cpg	307.04	J/mol×K	686.85	Joback Method
cpg	318.93	J/mol×K	729.81	Joback Method
cpg	329.93	J/mol×K	772.76	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=R640401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R640401&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>
<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>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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