

# 1,2-Dithiolane, 4-methyl

<b>Inchi:</b>	InChI=1S/C4H8S2/c1-4-2-5-6-3-4/h4H,2-3H2,1H3
<b>InchiKey:</b>	DAOKINZLHVYQX-UHFFFAOYSA-N
<b>Formula:</b>	C4H8S2
<b>SMILES:</b>	CC1CSSC1
<b>Mol. weight [g/mol]:</b>	120.24

## Physical Properties

Property code	Value	Unit	Source
gf	99.07	kJ/mol	Joback Method
hf	25.11	kJ/mol	Joback Method
hfus	7.36	kJ/mol	Joback Method
hvap	36.38	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	2.018		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
rinpol	1019.00		NIST Webbook
rinpol	1019.00		NIST Webbook
tb	401.86	K	Joback Method
tc	638.04	K	Joback Method
tf	312.64	K	Joback Method
vc	0.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.32	J/mol×K	401.86	Joback Method
cpg	160.81	J/mol×K	441.22	Joback Method
cpg	171.57	J/mol×K	480.59	Joback Method
cpg	181.64	J/mol×K	519.95	Joback Method
cpg	191.04	J/mol×K	559.31	Joback Method
cpg	199.83	J/mol×K	598.68	Joback Method
cpg	208.02	J/mol×K	638.04	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=R63085&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R63085&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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