

# 2,2,4-Trimethyl-1,3-dithiane

<b>Inchi:</b>	InChI=1S/C7H14S2/c1-6-4-5-8-7(2,3)9-6/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	FRRBWOYAAOXUHL-UHFFFAOYSA-N
<b>Formula:</b>	C7H14S2
<b>SMILES:</b>	CC1CCSC(C)(C)S1
<b>Mol. weight [g/mol]:</b>	162.32

## Physical Properties

Property code	Value	Unit	Source
gf	99.03	kJ/mol	Joback Method
hf	-48.07	kJ/mol	Joback Method
hfus	7.81	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.981		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	1200.00		NIST Webbook
tb	470.34	K	Joback Method
tc	716.10	K	Joback Method
tf	362.59	K	Joback Method
vc	0.450	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.58	J/mol×K	470.34	Joback Method
cpg	285.66	J/mol×K	511.30	Joback Method
cpg	301.45	J/mol×K	552.26	Joback Method
cpg	316.08	J/mol×K	593.22	Joback Method
cpg	329.73	J/mol×K	634.18	Joback Method
cpg	342.54	J/mol×K	675.14	Joback Method
cpg	354.65	J/mol×K	716.10	Joback Method

# Sources

<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=R155250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R155250&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccol:</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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