

# 1,4-Dithiane, 3,5-dimethyl, #1

Inchi:	InChI=1S/C6H12S2/c1-5-3-7-4-6(2)8-5/h5-6H,3-4H2,1-2H3
InchiKey:	VUMHVPHHEVBMOI-UHFFFAOYSA-N
Formula:	C6H12S2
SMILES:	CC1CSCC(C)S1
Mol. weight [g/mol]:	148.29

## Physical Properties

Property code	Value	Unit	Source
gf	96.10	kJ/mol	Joback Method
hf	-42.67	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	40.69	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.243		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
tb	447.22	K	Joback Method
tc	686.04	K	Joback Method
tf	327.42	K	Joback Method
vc	0.396	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.86	J/molxK	447.22	Joback Method
cpg	241.60	J/molxK	487.02	Joback Method
cpg	256.46	J/molxK	526.83	Joback Method
cpg	270.45	J/molxK	566.63	Joback Method
cpg	283.61	J/molxK	606.43	Joback Method
cpg	295.94	J/molxK	646.23	Joback Method
cpg	307.49	J/molxK	686.04	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=R82209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R82209&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>

# 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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