

# Thiolane, 2,3-dimethyl

<b>Inchi:</b>	InChI=1S/C6H12S/c1-5-3-4-7-6(5)2/h5-6H,3-4H2,1-2H3
<b>InchiKey:</b>	PQAQKWCWCGKBDS-UHFFFAOYSA-N
<b>Formula:</b>	C6H12S
<b>SMILES:</b>	CC1CCSC1C
<b>Mol. weight [g/mol]:</b>	116.22

## Physical Properties

Property code	Value	Unit	Source
gf	68.34	kJ/mol	Joback Method
hf	-81.77	kJ/mol	Joback Method
hfus	9.96	kJ/mol	Joback Method
hvap	34.71	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.148		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	899.00		NIST Webbook
tb	395.12	K	Joback Method
tc	607.56	K	Joback Method
tf	247.49	K	Joback Method
vc	0.357	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.26	J/mol×K	395.12	Joback Method
cpg	196.77	J/mol×K	430.53	Joback Method
cpg	210.55	J/mol×K	465.93	Joback Method
cpg	223.63	J/mol×K	501.34	Joback Method
cpg	236.02	J/mol×K	536.74	Joback Method
cpg	247.76	J/mol×K	572.15	Joback Method
cpg	258.85	J/mol×K	607.56	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R535770&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R535770&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>
<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>

# 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>rinpola:</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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