

# 1,2,3,4-Tetrathiepane

Inchi:	InChI=1S/C3H6S4/c1-2-4-6-7-5-3-1/h1-3H2
InchiKey:	XWJXXFXDJDNFKB-UHFFFAOYSA-N
Formula:	C3H6S4
SMILES:	C1CSSSSC1
Mol. weight [g/mol]:	170.34

## Physical Properties

Property code	Value	Unit	Source
gf	153.88	kJ/mol	Joback Method
hf	144.29	kJ/mol	Joback Method
hfus	6.82	kJ/mol	Joback Method
hvap	46.43	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.068		Crippen Method
mcvol	107.670	ml/mol	McGowan Method
pc	6229.41	kPa	Joback Method
rinpol	1375.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1371.00		NIST Webbook
tb	487.85	K	Joback Method
tc	788.29	K	Joback Method
tf	465.47	K	Joback Method
vc	0.314	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.05	J/molxK	487.85	Joback Method
cpg	194.41	J/molxK	537.92	Joback Method
cpg	204.79	J/molxK	588.00	Joback Method
cpg	214.24	J/molxK	638.07	Joback Method

cpg	222.81	J/mol×K	688.14	Joback Method
cpg	230.56	J/mol×K	738.22	Joback Method
cpg	237.53	J/mol×K	788.29	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R82085&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R82085&amp;Units=SI</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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