

# 3,5-dimethyl-1,2,4-trithiolane isomer

<b>Inchi:</b>	InChI=1S/C4H8S3/c1-3-5-4(2)7-6-3/h3-4H,1-2H3
<b>InchiKey:</b>	HFRUNLRFNNTTPQ-UHFFFAOYSA-N
<b>Formula:</b>	C4H8S3
<b>SMILES:</b>	CC1SSC(C)S1
<b>Mol. weight [g/mol]:</b>	152.30

## Physical Properties

Property code	Value	Unit	Source
gf	131.22	kJ/mol	Joback Method
hf	50.03	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	41.88	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.807		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
ripol	1604.00		NIST Webbook
tb	445.02	K	Joback Method
tc	698.77	K	Joback Method
tf	391.85	K	Joback Method
vc	0.338	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.82	J/mol×K	445.02	Joback Method
cpg	201.68	J/mol×K	487.31	Joback Method
cpg	212.78	J/mol×K	529.60	Joback Method
cpg	223.15	J/mol×K	571.90	Joback Method
cpg	232.82	J/mol×K	614.19	Joback Method
cpg	241.83	J/mol×K	656.48	Joback Method
cpg	250.21	J/mol×K	698.77	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=R301156&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R301156&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>

# 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>ripol:</b>	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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