

# 1,2,4-Trithiolane

<b>Inchi:</b>	InChI=1S/C2H4S3/c1-3-2-5-4-1/h1-2H2
<b>InchiKey:</b>	QHGFEUAAQKJXDI-UHFFFAOYSA-N
<b>Formula:</b>	C2H4S3
<b>SMILES:</b>	C1SCSS1
<b>Mol. weight [g/mol]:</b>	124.25
<b>CAS:</b>	289-16-7

## Physical Properties

Property code	Value	Unit	Source
gf	129.80	kJ/mol	Joback Method
hf	131.99	kJ/mol	Joback Method
hfus	4.77	kJ/mol	Joback Method
hvap	38.05	kJ/mol	Joback Method
ie	8.70 ± 0.20	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.030		Crippen Method
mcvol	77.230	ml/mol	McGowan Method
pc	6774.04	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1127.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1760.00		NIST Webbook
tb	408.60	K	Joback Method
tc	671.88	K	Joback Method
tf	377.79	K	Joback Method
vc	0.228	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.80	J/mol×K	408.60	Joback Method
cpg	122.51	J/mol×K	452.48	Joback Method
cpg	129.53	J/mol×K	496.36	Joback Method
cpg	135.92	J/mol×K	540.24	Joback Method
cpg	141.72	J/mol×K	584.12	Joback Method
cpg	147.00	J/mol×K	628.00	Joback Method
cpg	151.80	J/mol×K	671.88	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=C289167&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C289167&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>

## 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>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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

**vc:** Critical Volume

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