

# 2-tetrahydrothiophenethiol

<b>Inchi:</b>	InChI=1S/C4H8S2/c5-4-2-1-3-6-4/h4-5H,1-3H2
<b>InchiKey:</b>	MBURDTXKYKCZEZ-UHFFFAOYSA-N
<b>Formula:</b>	C4H8S2
<b>SMILES:</b>	SC1CCCS1
<b>Mol. weight [g/mol]:</b>	120.24

## Physical Properties

Property code	Value	Unit	Source
gf	88.60	kJ/mol	Joback Method
hf	18.33	kJ/mol	Joback Method
hfus	7.75	kJ/mol	Joback Method
hvap	37.30	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.769		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
rinqol	1017.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	416.89	K	Joback Method
tc	664.56	K	Joback Method
tf	265.65	K	Joback Method
vc	0.300	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.35	J/mol×K	416.89	Joback Method
cpg	163.41	J/mol×K	458.17	Joback Method
cpg	174.65	J/mol×K	499.45	Joback Method
cpg	185.12	J/mol×K	540.72	Joback Method
cpg	194.86	J/mol×K	582.00	Joback Method
cpg	203.90	J/mol×K	623.28	Joback Method
cpg	212.28	J/mol×K	664.56	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=R169269&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R169269&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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