

# 7-Thia-1-octanethiol

**Inchi:** InChI=1S/C7H16S2/c1-9-7-5-3-2-4-6-8/h8H,2-7H2,1H3  
**InchiKey:** MCCWTNNEODFSQN-UHFFFAOYSA-N  
**Formula:** C7H16S2  
**SMILES:** CSCCCCCCS  
**Mol. weight [g/mol]:** 164.33

## Physical Properties

Property code	Value	Unit	Source
gf	70.57	kJ/mol	Joback Method
hf	-107.46	kJ/mol	Joback Method
hfus	22.06	kJ/mol	Joback Method
hvap	44.73	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.840		Crippen Method
mvol	142.190	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
tb	491.20	K	Joback Method
tc	700.51	K	Joback Method
tf	239.51	K	Joback Method
vc	0.535	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.29	J/mol×K	491.20	Joback Method
cpg	307.70	J/mol×K	526.08	Joback Method
cpg	320.47	J/mol×K	560.97	Joback Method
cpg	332.63	J/mol×K	595.85	Joback Method
cpg	344.17	J/mol×K	630.74	Joback Method
cpg	355.13	J/mol×K	665.62	Joback Method
cpg	365.50	J/mol×K	700.51	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=R157672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R157672&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>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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