

# 5-Methyl-4-mercaptohexan-2-ol

**Inchi:** InChI=1S/C7H16OS/c1-5(2)7(9)4-6(3)8/h5-9H,4H2,1-3H3  
**InchiKey:** RTGGPWJVXQMFRP-UHFFFAOYSA-N  
**Formula:** C7H16OS  
**SMILES:** CC(O)CC(S)C(C)C  
**Mol. weight [g/mol]:** 148.27

## Physical Properties

Property code	Value	Unit	Source
gf	-106.69	kJ/mol	Joback Method
hf	-317.40	kJ/mol	Joback Method
hfus	11.45	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.712		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1124.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1762.00		NIST Webbook
tb	513.28	K	Joback Method
tc	703.28	K	Joback Method
tf	220.93	K	Joback Method
vc	0.482	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.66	J/mol×K	513.28	Joback Method
cpg	308.57	J/mol×K	544.95	Joback Method
cpg	319.93	J/mol×K	576.61	Joback Method
cpg	330.74	J/mol×K	608.28	Joback Method
cpg	341.03	J/mol×K	639.94	Joback Method
cpg	350.81	J/mol×K	671.61	Joback Method
cpg	360.09	J/mol×K	703.28	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=R282476&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R282476&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>
<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>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
<b>vc:</b>	Critical Volume

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