

# 5-Mercaptohexan-3-ol

Inchi:	InChI=1S/C6H14OS/c1-3-6(7)4-5(2)8/h5-8H,3-4H2,1-2H3
InchiKey:	CLTCBQPTBSNRIK-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	CCC(O)CC(C)S
Mol. weight [g/mol]:	134.24

## Physical Properties

Property code	Value	Unit	Source
gf	-112.67	kJ/mol	Joback Method
hf	-291.48	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.466		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1049.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	490.84	K	Joback Method
tc	679.02	K	Joback Method
tf	224.66	K	Joback Method
vc	0.432	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.45	J/mol×K	490.84	Joback Method
cpg	264.05	J/mol×K	522.20	Joback Method
cpg	274.16	J/mol×K	553.57	Joback Method
cpg	283.81	J/mol×K	584.93	Joback Method
cpg	293.00	J/mol×K	616.29	Joback Method
cpg	301.75	J/mol×K	647.66	Joback Method
cpg	310.08	J/mol×K	679.02	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=R282461&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R282461&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>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
<b>vc:</b>	Critical Volume

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