

# 7-Mercaptoheptanol

Inchi:	InChI=1S/C7H16OS/c8-6-4-2-1-3-5-7-9/h8-9H,1-7H2
InchiKey:	LSLIREXBGQDXDX-UHFFFAOYSA-N
Formula:	C7H16OS
SMILES:	OCCCCCCCS
Mol. weight [g/mol]:	148.27

## Physical Properties

Property code	Value	Unit	Source
gf	-99.37	kJ/mol	Joback Method
hf	-301.56	kJ/mol	Joback Method
hfus	22.02	kJ/mol	Joback Method
hvap	54.59	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.859		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
ripol	2083.00		NIST Webbook
tb	514.60	K	Joback Method
tc	693.27	K	Joback Method
tf	265.93	K	Joback Method
vc	0.500	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.82	J/mol×K	514.60	Joback Method
cpg	306.83	J/mol×K	544.38	Joback Method
cpg	317.37	J/mol×K	574.16	Joback Method
cpg	327.45	J/mol×K	603.94	Joback Method
cpg	337.08	J/mol×K	633.71	Joback Method
cpg	346.28	J/mol×K	663.49	Joback Method
cpg	355.06	J/mol×K	693.27	Joback Method

# Sources

<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>
<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=R568780&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R568780&amp;Units=SI</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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