

# 4-mercaptopentane-2-ol

<b>Other names:</b>	4-mercaptopentane-2-one 4-mercapto-2-pentanone
<b>Inchi:</b>	InChI=1S/C5H10OS/c1-4(6)3-5(2)7/h5,7H,3H2,1-2H3
<b>InchiKey:</b>	KHIPEWLRUGVKIC-UHFFFAOYSA-N
<b>Formula:</b>	C5H10OS
<b>SMILES:</b>	CC(=O)CC(C)S
<b>Mol. weight [g/mol]:</b>	118.20

## Physical Properties

Property code	Value	Unit	Source
gf	-110.75	kJ/mol	Joback Method
hf	-225.91	kJ/mol	Joback Method
hfus	10.82	kJ/mol	Joback Method
hvap	39.82	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.284		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	884.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1587.00		NIST Webbook
tb	430.09	K	Joback Method
tc	638.12	K	Joback Method
tf	217.50	K	Joback Method
vc	0.369	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.43	J/mol×K	430.09	Joback Method
cpg	193.22	J/mol×K	464.76	Joback Method
cpg	202.55	J/mol×K	499.43	Joback Method
cpg	211.43	J/mol×K	534.10	Joback Method
cpg	219.86	J/mol×K	568.78	Joback Method
cpg	227.86	J/mol×K	603.45	Joback Method
cpg	235.44	J/mol×K	638.12	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R202801&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202801&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>
<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>

## 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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