

# Cyclopentanethiol, 1-methyl-

<b>Other names:</b>	1-Methylcyclopentanethiol
<b>Inchi:</b>	InChI=1S/C6H12S/c1-6(7)4-2-3-5-6/h7H,2-5H2,1H3
<b>InchiKey:</b>	XJWBHFDHEOPYNK-UHFFFAOYSA-N
<b>Formula:</b>	C6H12S
<b>SMILES:</b>	CC1(S)CCCC1
<b>Mol. weight [g/mol]:</b>	116.22
<b>CAS:</b>	1638-95-5

## Physical Properties

Property code	Value	Unit	Source
gf	60.09	kJ/mol	Joback Method
hf	-52.97	kJ/mol	Joback Method
hfus	2.97	kJ/mol	Joback Method
hvap	34.79	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.249		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	410.75 ± 0.20	K	NIST Webbook
tc	649.06	K	Joback Method
tf	228.64	K	Joback Method
vc	0.364	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.32	J/mol×K	415.06	Joback Method
cpg	201.81	J/mol×K	454.06	Joback Method
cpg	215.98	J/mol×K	493.06	Joback Method
cpg	228.97	J/mol×K	532.06	Joback Method
cpg	240.91	J/mol×K	571.06	Joback Method
cpg	251.97	J/mol×K	610.06	Joback Method
cpg	262.27	J/mol×K	649.06	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1638955&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1638955&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>
<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>hvp:</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>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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