

# 2-Pentanethiol, 4-methyl-

<b>Inchi:</b>	InChI=1S/C6H14S/c1-5(2)4-6(3)7/h5-7H,4H2,1-3H3
<b>InchiKey:</b>	JBCIMWBQDMBMMP-UHFFFAOYSA-N
<b>Formula:</b>	C6H14S
<b>SMILES:</b>	CC(C)CC(C)S
<b>Mol. weight [g/mol]:</b>	118.24
<b>CAS:</b>	1639-05-0

## Physical Properties

Property code	Value	Unit	Source
gf	24.15	kJ/mol	Joback Method
hf	-139.25	kJ/mol	Joback Method
hfus	8.29	kJ/mol	Joback Method
hvap	34.91	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.351		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	398.66	K	Joback Method
tc	596.55	K	Joback Method
tf	163.84	K	Joback Method
vc	0.413	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.76	J/mol×K	398.66	Joback Method
cpg	217.01	J/mol×K	431.64	Joback Method
cpg	228.72	J/mol×K	464.62	Joback Method
cpg	239.90	J/mol×K	497.61	Joback Method
cpg	250.57	J/mol×K	530.59	Joback Method
cpg	260.75	J/mol×K	563.57	Joback Method
cpg	270.44	J/mol×K	596.55	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C1639050&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1639050&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>mccvol:</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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