

# 2-mercapto-3-methylbutanol

<b>Other names:</b>	2-mercapto-3-methyl-1-butanol
<b>Inchi:</b>	InChI=1S/C5H12OS/c1-4(2)5(7)3-6/h4-7H,3H2,1-2H3
<b>InchiKey:</b>	QBYYSQQYPUMFOX-UHFFFAOYSA-N
<b>Formula:</b>	C5H12OS
<b>SMILES:</b>	CC(C)C(S)CO
<b>Mol. weight [g/mol]:</b>	120.21

## Physical Properties

Property code	Value	Unit	Source
gf	-121.09	kJ/mol	Joback Method
hf	-270.84	kJ/mol	Joback Method
hfus	9.79	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.933		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1656.00		NIST Webbook
tb	467.96	K	Joback Method
tc	658.24	K	Joback Method
tf	213.39	K	Joback Method
vc	0.377	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.56	J/mol×K	467.96	Joback Method
cpg	222.02	J/mol×K	499.67	Joback Method
cpg	231.06	J/mol×K	531.39	Joback Method

cpg	239.68	J/mol×K	563.10	Joback Method
cpg	247.90	J/mol×K	594.82	Joback Method
cpg	255.72	J/mol×K	626.53	Joback Method
cpg	263.16	J/mol×K	658.24	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=R423979&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R423979&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>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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