

# 4,4-Dimethyl-3-thia-1-pentanethiol

<b>Inchi:</b>	InChI=1S/C6H14S2/c1-6(2,3)8-5-4-7/h7H,4-5H2,1-3H3
<b>InchiKey:</b>	WBOABOGBRQWNPV-UHFFFAOYSA-N
<b>Formula:</b>	C6H14S2
<b>SMILES:</b>	CC(C)(C)SCCS
<b>Mol. weight [g/mol]:</b>	150.31

## Physical Properties

Property code	Value	Unit	Source
gf	64.99	kJ/mol	Joback Method
hf	-95.57	kJ/mol	Joback Method
hfus	12.05	kJ/mol	Joback Method
hvap	41.21	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.448		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinsol	1105.00		NIST Webbook
tb	465.09	K	Joback Method
tc	692.23	K	Joback Method
tf	230.66	K	Joback Method
vc	0.469	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.25	J/mol×K	465.09	Joback Method
cpg	268.76	J/mol×K	502.95	Joback Method
cpg	281.43	J/mol×K	540.80	Joback Method
cpg	293.31	J/mol×K	578.66	Joback Method
cpg	304.43	J/mol×K	616.52	Joback Method
cpg	314.82	J/mol×K	654.37	Joback Method
cpg	324.52	J/mol×K	692.23	Joback Method

# Sources

<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=R156951&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R156951&amp;Units=SI</a>
<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>

# 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>rinpola:</b>	Non-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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